STIC Search Report

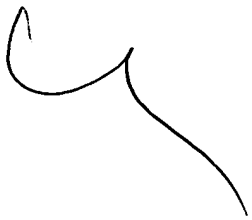
Biotech-Chem Library

STIC Database Tracking Number: 111586

TO: Michael Lavilla Location: REM 5e79 Thursday, January 08, 2004 Art Unit: 1775 Phone: 571-272-1539 Serial Number: 09 / 700821	From: Jan Delaval Location: Biotech-Chem Library Remsen Building – 1A51 Phone: 571-272-2504 jan.delaval@uspto.gov

Search Notes

10/6/2000



Search and Information Resources Administration

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=> fil reg
FILE 'REGISTRY' ENTERED AT 07:55:34 ON 08 JAN 2004
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STRUCTURE FILE UPDATES:    6 JAN 2004  HIGHEST RN 634878-43-6
DICTIONARY FILE UPDATES:   6 JAN 2004  HIGHEST RN 634878-43-6

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que l16
L7              STR
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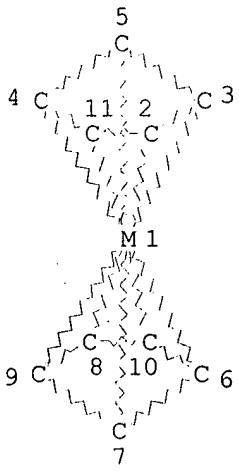


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NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  11

STEREO ATTRIBUTES: NONE
L9              SCR 2017
L11         7674 SEA FILE=REGISTRY SSS FUL L7 AND L9
L12          423 SEA FILE=REGISTRY ABB=ON  PLU=ON  L11 AND (FE AND RH)/ELS
L13             STR
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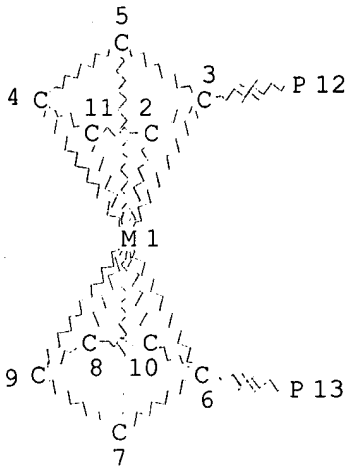


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L15        3743 SEA FILE=REGISTRY SUB=L11 SSS FUL L13
L16         265 SEA FILE=REGISTRY ABB=ON  PLU=ON  L12 AND L15

=> d his

     (FILE 'HOME' ENTERED AT 07:07:27 ON 08 JAN 2004)
               SET COST OFF

     FILE 'HCAPLUS' ENTERED AT 07:07:47 ON 08 JAN 2004
L1             1 S (WO2000-GB3851 OR GB99-23952)/AP,PRN
               E BURK M/AU
L2           127 S E3,E5,E11-E13
               E GERLACH A/AU
L3            50 S E3,E4,E21
               E CHIROTECH/PA,CS
L4           213 S E3-E31
               SEL RN L1

     FILE 'REGISTRY' ENTERED AT 07:10:11 ON 08 JAN 2004
L5             9 S E1-E9
               E FERROCENE/CN
L6             1 S E3
L7               STR
L8            50 S L7
L9               SCR 2017
L10           50 S L7 AND L9
L11         7674 S L7 AND L9 FUL
               SAV L11 LAVILLA700/A
L12          423 S L11 AND (FE AND RH)/ELS
L13              STR L7
L14           50 S L13 SAM SUB=L11
L15         3743 S L13 FUL SUB=L11
               SAV L15 LAVILLA700A/A
L16          265 S L12 AND L15
```

```
L17             STR L13
L18           3 S L17 SAM SUB=L15
L19         142 S L17 FUL SUB=L15
                SAV L19 LAVILLA700B/A
L20          26 S L16 AND L19
L21          20 S L20 AND 1/RH
L22          16 S L21 AND 2/P AND 1/FE
L23           4 S L21 NOT L22
L24          15 S L22 NOT C27H37F6FEO2P2RH

     FILE 'HCAOLD' ENTERED AT 07:20:25 ON 08 JAN 2004
L25           0 S L24

     FILE 'USPATFULL, USPAT2' ENTERED AT 07:20:29 ON 08 JAN 2004
L26           0 S L24

     FILE 'HCAPLUS' ENTERED AT 07:20:33 ON 08 JAN 2004
L27          15 S L24
L28           5 S L27 AND L1-L4
                E ALDEHYDE/CT
L29      386960 S E17+NT
L30       48009 S E3-E67
L31      502889 S ?ALDEHYD?
L32        1876 S L15
                E HYDROGENATION/CT
L33       46596 S E3+NT
L34       36933 S E20+NT
L35         132 S E32+NT
L36        1397 S E36+NT
L37         104 S L16
L38          22 S L37 AND L29-L31
L39           7 S L38 AND L33-L36
L40           8 S L38 AND ?ALCOHOL?
L41           4 S L39 AND L40
L42          11 S L28,L39-L41
L43           1 S L27 AND P/DT
L44          21 S L27,L42,L43
L45          17 S L44 AND ?HYDROGENAT?
L46           9 S L45 AND L29-L31
L47           9 S L28,L46
L48          12 S L44,L45 NOT L47
                SEL HIT RN L48

     FILE 'REGISTRY' ENTERED AT 07:35:33 ON 08 JAN 2004
L49          13 S E1-E13
L50          10 S L49 AND L11

     FILE 'HCAPLUS' ENTERED AT 07:36:42 ON 08 JAN 2004
L51          18 S L50
L52          15 S L51 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
L53           4 S L47 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
L54          19 S L28,L52,L53
L55          19 S L54 AND L1-L4,L27-L48,L51-L54
L56        4071 S PHOSPHOTUNGSTIC ACID
L57        2345 S PHOSPHOMOLYBDIC ACID
L58        1136 S SILICOTUNGSTIC ACID

     FILE 'REGISTRY' ENTERED AT 07:39:46 ON 08 JAN 2004
L59           3 S 1343-93-7 OR 12026-57-2 OR 12027-38-2
L60           3 S 12534-77-9 OR 12379-13-4 OR 12363-31-4
L61        1638 S (12534-77-9 OR 12379-13-4 OR 12363-31-4)/CRN

     FILE 'HCAPLUS' ENTERED AT 07:41:13 ON 08 JAN 2004
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L62         3445 S L59 OR L60
L63         4365 S L61
L64            3 S L56-L58,L62-L63 AND L37
L65            2 S L16 AND ALUMINA

     FILE 'REGISTRY' ENTERED AT 07:42:26 ON 08 JAN 2004
L66            1 S 1344-28-1

     FILE 'HCAPLUS' ENTERED AT 07:42:40 ON 08 JAN 2004
L67       218225 S L66
L68       342015 S AL2O3 OR ALUMINUM OXIDE
L69            2 S L67,L68 AND L16
L70            0 S TETRAFLUOROETHYLENE PERFLUORO VINYL ETHER SULFONATE
L71            0 S TETRAFLUOROETHYLENE PERFLUORO VINYL ETHER SULPHONATE
L72            0 S TETRAFLUOROETHYLENE PERFLUOROVINYL ETHER SULPHONATE
L73            0 S TETRAFLUOROETHYLENE PERFLUOROVINYL ETHER SULFONATE
L74            0 S ?TETRAFLUOROETHYLENE? AND L16
L75            6 S ?VINYL? AND L16
L76          163 S ?TETRAFLUOROETHYLEN? (L) ?VINYL? (L) (?SULFONATE? OR ?SULPHON
L77        23774 S PTFE
L78           60 S L77 (L) ?VINYL? (L) (?SULFONATE? OR ?SULPHONATE?)

     FILE 'REGISTRY' ENTERED AT 07:47:13 ON 08 JAN 2004
L79            1 S 9002-84-0
L80            1 S 116-14-3
L81         3998 S 116-14-3/CRN
L82          412 S L81 AND S/ELS
L83           76 S L82 AND NR>=1
L84          336 S L82 NOT L83
L85          247 S L84 NOT N/ELS
L86           97 S L85 AND 2/NC
L87          127 S L85 AND 3/NC
L88           23 S L85 NOT L86,L87
L89          244 S L85 NOT SI/ELS

     FILE 'HCAPLUS' ENTERED AT 07:52:06 ON 08 JAN 2004
L90            0 S L89 AND L16
L91            0 S L79,L80 AND L16
L92            0 S L82 AND L16
L93           19 S L64,L65,L69,L55

     FILE 'REGISTRY' ENTERED AT 07:53:24 ON 08 JAN 2004

     FILE 'HCAPLUS' ENTERED AT 07:53:31 ON 08 JAN 2004
L94           19 S L93 AND (RH OR ?RHODIUM?)

     FILE 'REGISTRY' ENTERED AT 07:55:34 ON 08 JAN 2004

     FILE 'HCAPLUS' ENTERED AT 07:55:42 ON 08 JAN 2004
               SEL HIT RN L94

     FILE 'REGISTRY' ENTERED AT 07:57:38 ON 08 JAN 2004
L95           59 S E14-E72
L96           31 S L16 AND L95
L97           28 S L95 NOT L96
L98           12 S L97 AND L11
L99           16 S L97 NOT L98

     FILE 'HCAPLUS' ENTERED AT 07:59:28 ON 08 JAN 2004
L100          26 S L96
L101          20 S L100 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
L102          16 S L101 AND L94
L103           4 S L101 NOT L102
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L104 20 S L101-L103

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 08:01:16 ON 08 JAN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 8 Jan 2004 VOL 140 ISS 2
FILE LAST UPDATED: 6 Jan 2004 (20040106/ED)

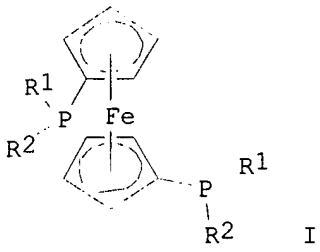
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l104 all hitstr tot

L104 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:283853 HCAPLUS
DN 134:312797
ED Entered STN: 20 Apr 2001
TI Supported ferrocene-based catalysts for selective **aldehyde hydrogenation**
IN **Burk, Mark Joseph; Gerlach, Arne**
PA **Chirotech Technology Limited, UK**
SO PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DT **Patent**
LA English
IC ICM B01J031-22
ICS B01J031-28; C07C045-62
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 67
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001026807	A1	20010419	WO 2000-GB3851	20001006 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1222026	A1	20020717	EP 2000-964538	20001006 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2003511229	T2	20030325	JP 2001-529860	20001006 <--
PRAI	GB 1999-23952	A	19991008 <--		
	WO 2000-GB3851	W	20001006 <--		

OS MARPAT 134:312797
GI



I

AB A supported catalyst comprises a cationic **rhodium** (I) complex of formula I, wherein R1 and R2 are the same or different C≤30 hydrocarbyl groups, or R1 and R2 are linked to form a ring, and a heterogeneous support medium that provides anionic binding sites. Such a complex is particularly useful as a catalyst in a process of **hydrogenating** an **aldehyde** to produce the corresponding primary **alc.** Stirring 288 mg **phosphotungstic acid** with 4 g silica gel for 1 h, stirring the mixture with 64 mg [(DiPFc)**Rh**(COD)]BF4 (COD = cyclooctadiene; DiPFc 1,1'-bis(disiopropylphosphino)ferrocene) gave a catalyst, which reduced pentanal to pentanol in 100% yield.

ST supported ferrocene catalyst selective **aldehyde hydrogenation**; pentanal **hydrogenation** catalyst **rhodium** ferrocene complex

IT Metallocenes
RL: CAT (Catalyst use); USES (Uses)
(ferrocenes; supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT **Alcohols**, preparation
RL: IMF (Industrial manufacture); PREP (Preparation)
(primary; supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT **Hydrogenation catalysts**
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT **Aldehydes, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT **255064-36-9**
RL: CAT (Catalyst use); USES (Uses)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT 7440-16-6DP, **Rhodium**, complex with 1,1'-bis(diisopropylphosphino)ferrocene, preparation **97239-80-0DP**, 1,1'-Bis(diisopropylphosphino)ferrocene, **rhodium** complex
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT 71-41-0P, n-Pentanol, preparation 505-10-2P 619-73-8P, p-Nitrobenzyl **alcohol** 636-72-6P, Thiophene-2-methanol 873-75-6P, p-Bromobenzyl **alcohol** 3446-90-0P, p-Methylthiobenzyl **alcohol** 6214-45-5P, p-Butoxybenzyl **alcohol** 79757-77-0P, 4-Bromo-Thiophene-2-methanol

RL: IMF (Industrial manufacture); PREP (Preparation)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT **98-03-3**, 2-Formylthiophene **110-62-3**, Pentanal
555-16-8, p-**Nitrobenzaldehyde**, reactions
1122-91-4, p-**Bromobenzaldehyde** **3268-49-3**
3446-89-7, p-**Thiomethylbenzaldehyde** 5736-88-9, p-**Butoxybenzaldehyde** 18791-75-8, 4-Bromo-2-Formylthiophene
RL: RCT (Reactant); RACT (Reactant or reagent)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

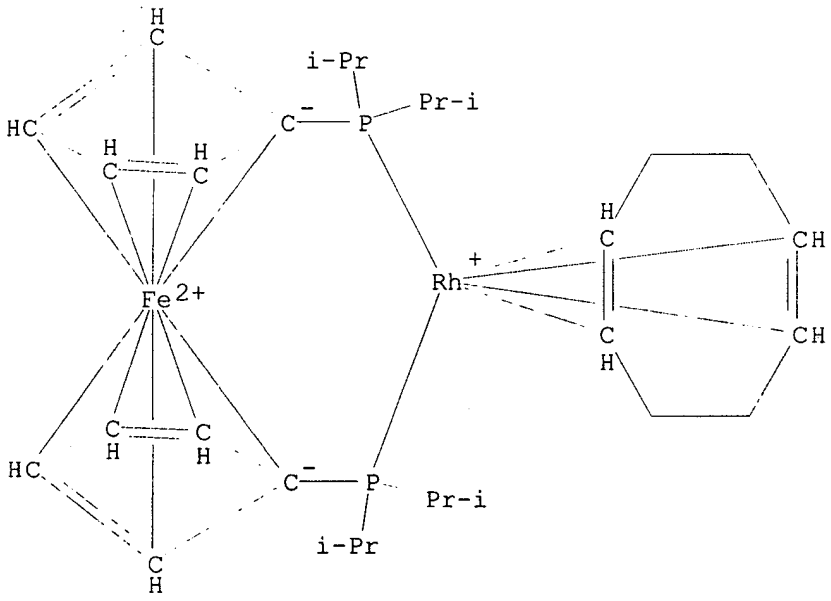
(1) Burk, M; TETRAHEDRON LETTERS 1994, V35(28), P4963 HCAPLUS
(2) Pugin, B; US 5783715 A 1998 HCAPLUS
(3) Seton Hall University; WO 9828074 A 1998 HCAPLUS

IT **255064-36-9**
RL: CAT (Catalyst use); USES (Uses)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

RN 255064-36-9 HCAPLUS
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

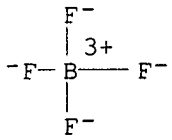
CM 1

CRN 157772-65-1
CMF C30 H48 Fe P2 Rh
CCI CCS

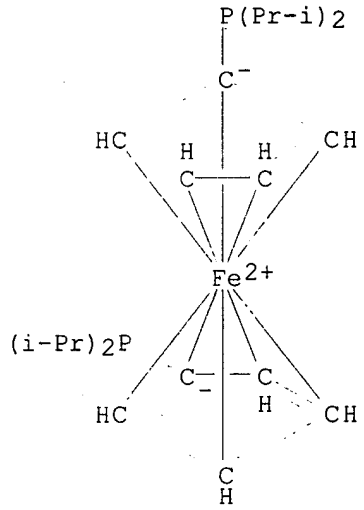


CM 2

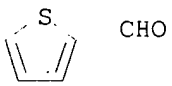
CRN 14874-70-5
CMF B F4
CCI CCS



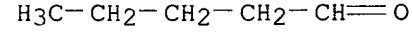
IT **97239-80-0DP**, 1,1'-Bis(diisopropylphosphino)ferrocene, **rhodium** complex
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)
RN 97239-80-0 HCAPLUS
CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphino]- (9CI) (CA INDEX NAME)



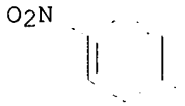
IT **98-03-3**, 2-Formylthiophene **110-62-3**, Pentanal
555-16-8, p-**Nitrobenzaldehyde**, reactions
1122-91-4, p-**Bromobenzaldehyde** **3268-49-3**
3446-89-7, p-**Thiomethylbenzaldehyde**
RL: RCT (Reactant); RACT (Reactant or reagent)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)
RN 98-03-3 HCAPLUS
CN 2-Thiophenecarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



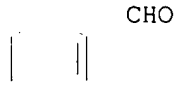
RN 110-62-3 HCAPLUS
CN Pentanal (9CI) (CA INDEX NAME)



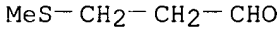
RN 555-16-8 HCAPLUS
CN Benzaldehyde, 4-nitro- (9CI) (CA INDEX NAME)



RN 1122-91-4 HCAPLUS
CN Benzaldehyde, 4-bromo- (9CI) (CA INDEX NAME)



RN 3268-49-3 HCAPLUS
CN Propanal, 3-(methylthio)- (9CI) (CA INDEX NAME)



RN 3446-89-7 HCAPLUS
CN Benzaldehyde, 4-(methylthio)- (9CI) (CA INDEX NAME)

L104 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:767776 HCAPLUS
DN 132:108089
ED Entered STN: 06 Dec 1999
TI Phosphines versus phosphinites as ligands in the **rhodium** catalyzed asymmetric **hydrogenation** of imines: a systematic study
AU Tararov, Vitali I.; Kadyrov, Renat; Riermeier, Thomas H.; Holz, Jens; Borner, Armin
CS Institut fur Organische Katalyseforschung an der Universitat Rostock e.V., Rostock, D-18055, Germany
SO Tetrahedron: Asymmetry (**1999**), 10(20), 4009-4015
CODEN: TASYE3; ISSN: 0957-4166
PB Elsevier Science Ltd.
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 67
OS CASREACT 132:108089
AB The asym. **hydrogenation** of N-(1-phenylethylidene)benzylamine with a range of **Rh**(I)-diphosphine and diphosphinite catalysts was studied. The reaction is strongly sensitive to the size of the metal chelate. Complexes based on five- and six-membered chelates or electron-rich alkylphosphines gave poor or moderate conversions. The reactivity of diphosphine catalysts could be increased by the addition of p-toluenesulfonic acid. Unexpectedly, **Rh**-complexes based on chiral diphosphinites and a diphosphite also rapidly converted the substrate to the desired amine. Highest efficiency was observed with a

Rh(I) complex with (R,R)-1,2-cyclohexanol-bisdiphenylphosphinite [(R,R)-bdpch] as chiral ligand. Without any additive complete **hydrogenation** of the imine was achieved within 5 h. The product was produced in an enantioselectivity of 71%.

ST phosphine phosphinite ligand comparison **rhodium** catalyzed asym **hydrogenation** imine

IT Phosphines
RL: CAT (Catalyst use); USES (Uses)
(diphosphines; phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT Amines, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines)

IT Imines
RL: RCT (Reactant); RACT (Reactant or reagent)
(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT **Hydrogenation**
Hydrogenation catalysts
(stereoselective; phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT 14428-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(: (phosphine)- and (phosphinite)**rhodium**-catalyzed asym. **hydrogenation** of)

IT 53450-79-6 60104-68-9 60430-43-5 63569-12-0 66787-44-8
72611-80-4 79255-71-3 82796-32-5 109143-86-4 163161-28-2
171561-30-1 171561-32-3 180420-80-8 185754-11-4 187886-92-6
204762-36-7 214827-80-2 217818-18-3 237058-40-1 255064-34-7
255064-35-8 255064-36-9 255064-38-1 255064-68-7
255719-90-5
RL: CAT (Catalyst use); USES (Uses)
(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines)

IT 17480-69-2P 38235-77-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Achiwa, K; J Am Chem Soc 1976, V98, P8265 HCAPLUS
(2) Bakos, J; J Chem Soc, Chem Commun 1991, P1684 HCAPLUS
(3) Bomer, A; Tetrahedron Lett 1994, V35, P6071
(4) Borns, S; Eur J Inorg Chem 1998, P1291 HCAPLUS
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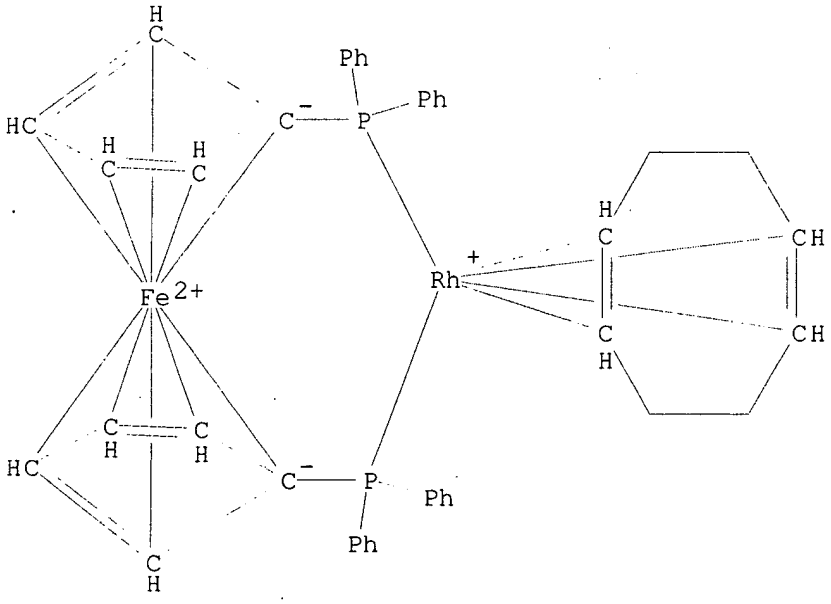
IT **255064-35-8 255064-36-9**
RL: CAT (Catalyst use); USES (Uses)
(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines)

RN 255064-35-8 HCAPLUS
CN Rhodium(1+), [1,1'-bis(diphenylphosphino-κP)ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

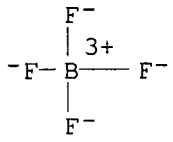
CRN 91159-09-0
CMF C42 H40 Fe P2 Rh
CCI CCS



CM 2

CRN 14874-70-5
CMF B F4

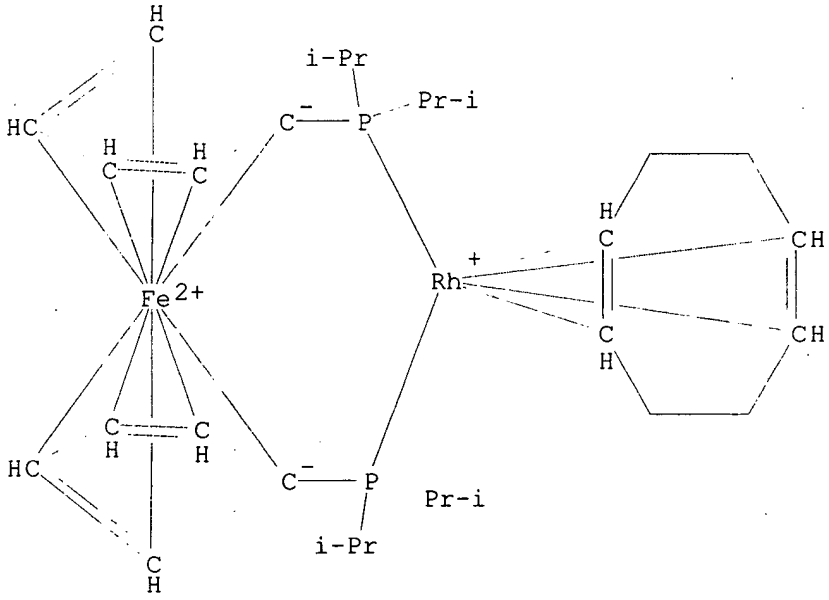
CCI CCS



RN 255064-36-9 HCAPLUS
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

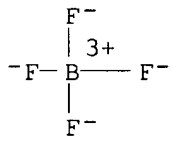
CM 1

CRN 157772-65-1
CMF C30 H48 Fe P2 Rh
CCI CCS



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



L104 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:668047 HCAPLUS

DN 129:303986
ED Entered STN: 22 Oct 1998
TI Processes and catalysts for producing **hydroxyaldehydes**
IN Briggs, John Robert; Packett, Diane Lee; Bryant, David Robert; Phillips, Ailene Gardner; Schreck, David James; Olson, Kurt Damar; Tjaden, Erik Bruce; Guram, Anil Sakharam; Eisenschmid, Thomas Carl; Brigham, Elaine Susan
PA Union Carbide Chemicals & Technology Corp., USA
SO U.S., 36 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07C045-50
NCL 568454000
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5821389	A	19981013	US 1997-843339	19970415 <--
	CN 1222903	A	19990714	CN 1997-195721	19970423 <--
PRAI	US 1997-843339		19970415 <--		

OS MARPAT 129:303986
AB This invention relates in part to processes for producing one or more substituted or unsubstituted **hydroxyaldehydes**, e.g., 6-hydroxyhexanals, which comprise subjecting one or more substituted or unsubstituted alkadienes, e.g., butadiene, to reductive hydroformylation in the presence of a reductive hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, and hydroformylation in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, to produce one or more substituted or unsubstituted **hydroxyaldehydes**. The substituted and unsubstituted **hydroxyaldehydes** produced by the processes of this invention can undergo further reaction(s) to afford desired derivs. thereof, e.g., epsilon caprolactone. This invention also relates in part to reaction mixts. containing one or more substituted or unsubstituted **hydroxyaldehydes** as principal product(s) of reaction.
ST **hydroxyaldehyde** manuf diene hydroformylation; metal organophosphorus ligand complex catalyst hydroformylation
IT **Aldehydes, preparation**
RL: IMF (Industrial manufacture); PREP (Preparation)
(**hydroxy**; processes and catalysts for producing **hydroxyaldehydes**)
IT Hydroformylation
Hydroformylation catalysts
(processes and catalysts for producing **hydroxyaldehydes**)
IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)
(processes and catalysts for producing **hydroxyaldehydes**)
IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses 607-01-2, Ethyldiphenylphosphine 998-40-3, Tributylphosphine 1605-53-4, Diethylphenylphosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 4706-17-6 4731-53-7, Trioctylphosphine 6372-40-3, Isopropyldiphenylphosphine 6737-42-4 **12150-46-8** 14874-82-9, **Rhodium** dicarbonyl acetylacetonate 17005-57-1 19262-01-2, Cyclohexyldiethylphosphine 32305-98-9 32376-20-8, t-Butyldiethylphosphine 50420-43-4, n-Butyldiethylphosphine 53111-20-9, Diphenyl(o-methoxyphenyl)phosphine 76189-55-4, (R)-(+)-2,2'-Bis(diphenylphosphino)-1,1'-binaphthyl **84680-96-6** 108793-33-5 111982-81-1, 2,2'-(Bisdiphenylphosphinomethyl)1,1'-biphenyl 121627-17-6 138776-88-2 138776-89-3 154813-98-6 154814-02-5 169254-16-4 198475-94-4 198478-30-7 198478-33-0
RL: CAT (Catalyst use); USES (Uses)
(processes and catalysts for producing **hydroxyaldehydes**)

IT 34067-76-0P, 6-Hydroxyhexanal
RL: IMF (Industrial manufacture); PREP (Preparation)
(processes and catalysts for producing **hydroxyaldehydes**)
IT 764-37-4P, trans-3-Penten-1-ol 764-38-5P, cis-3-Penten-1-ol 821-09-0P, 4-Penten-1-ol 1576-95-0P, cis-2-Penten-1-ol 1576-96-1P, trans-2-Penten-1-ol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(processes and catalysts for producing **hydroxyaldehydes**)
IT 106-99-0, Butadiene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(processes and catalysts for producing **hydroxyaldehydes**)
RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(14) Dennis; US 4567306 1996 HCAPLUS
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(36) Smith; US 4224255 1980 HCAPLUS
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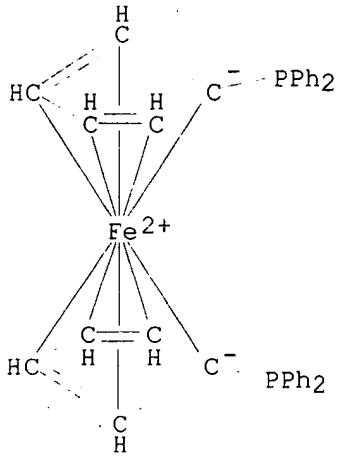
(39) Yates; US 4443638 1984 HCAPLUS
(40) Young; US 4625068 1986 HCAPLUS
IT **12150-46-8 84680-96-6**
RL: CAT (Catalyst use); USES (Uses)
(processes and catalysts for producing **hydroxyaldehydes**)
RN 12150-46-8 HCAPLUS
CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



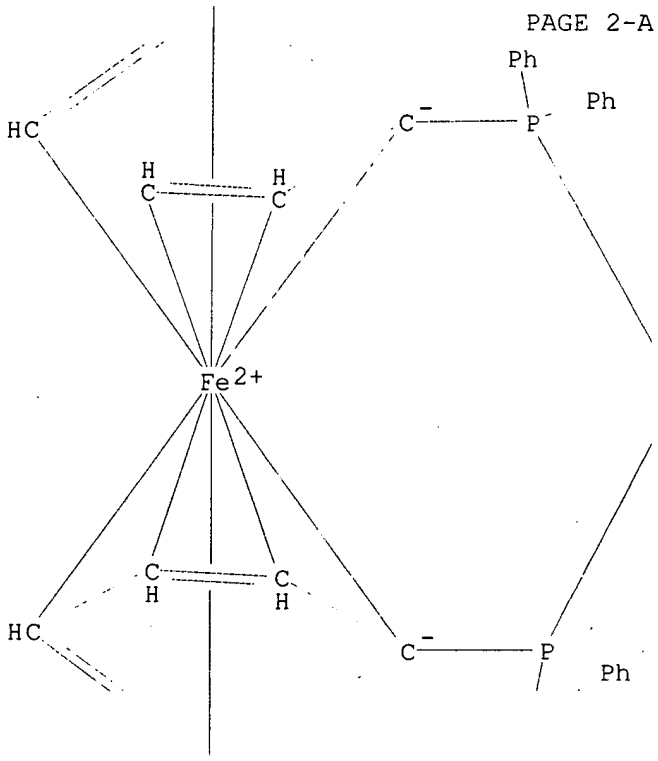
RN 84680-96-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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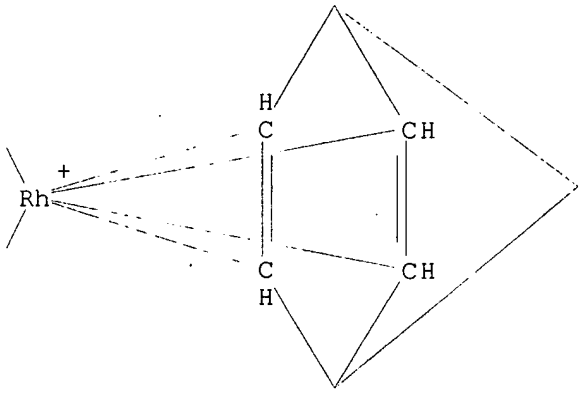
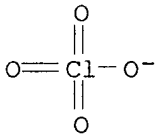


PAGE 3-A
Ph

CM 2

CRN 14797-73-0
CMF Cl O4



L104 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:756953 HCAPLUS
DN 128:14354
ED Entered STN: 04 Dec 1997
TI Selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor
IN Packett, Diane Lee; Briggs, John Robert; Bryant, David Robert; Phillips, Ailene Gardner
PA Union Carbide Chemicals and Plastics Technology Corp., USA
SO PCT Int. Appl., 109 pp.
CODEN: PIXXD2
DT Patent
LA English
IC C07C045-49; C07C047-21; C07C029-141; C07C033-025
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67
FAN.CNT 7

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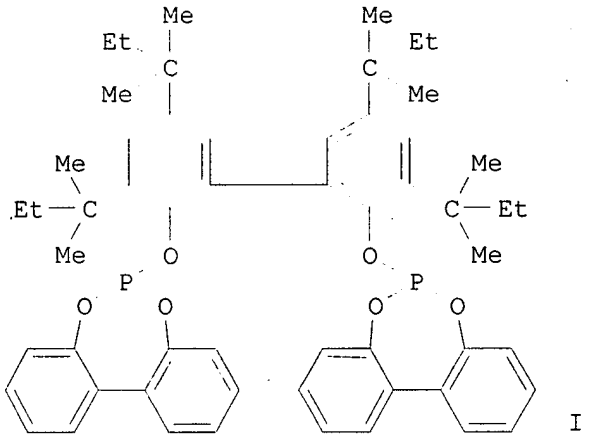
	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5886237	A	19990323	US 1997-843389	19970415 <--
	US 6187970	B1	20010213	US 1997-843390	19970415 <--
	AU 9727422	A1	19971112	AU 1997-27422	19970423 <--
	EP 853609	A1	19980722	EP 1997-921365	19970423 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PRAI	US 1996-15944P	P	19960424 <--		
	US 1996-15953P	P	19960424 <--		
	US 1996-16116P	P	19960424 <--		
	US 1996-16287P	P	19960424 <--		
	US 1997-843389	A	19970415 <--		

US 1997-842665 A 19970415 <--
WO 1997-US6889 W 19970423 <--
OS MARPAT 128:14354
GI



I

AB Substituted or unsubstituted alkadienes, e.g., butadiene, or a mixture thereof are hydroformylated in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, and at an alkadiene and/or carbon monoxide partial pressure sufficient to selectively produce ≥1 (un)substituted alkenal, e.g., pentenal. The (un)substituted alkenals can undergo further reaction(s) to afford desired derivs., e.g., **hydrogenation** to alkenols, particularly pentenols. The invention also relates to reaction mixts. containing ≥1 (un)substituted alkenals or alkenols as principal product(s) of the reactions. Thus, liquid butadiene was charged to a reactor containing a THF solution of **rhodium** dicarbonylacetylacetonate (200 ppm **Rh**) and 6,6'-[[3,3',5,5'-tetrakis(1,1-dimethylpropyl)-[1,1'-biphenyl]-1,1'-diyl]bis(oxy)]bis-dibenzo[d,f][1,3,2]dioxaphosphepin (I) (12:1 ligand-**Rh** ratio), heated to 95° and pressurized to 500 psig with 1:1 CO-H2 to give, after 2 h, 95% butadiene conversion to 3-pentenals 75, 4-pentenal 3, 2-pentenals 5, **valeraldehyde** 7, branched **dialdehyde** 1, and **adipaldehyde** 9%.

ST alkadiene hydroformylation alkenal alkenol manuf; butadiene hydroformylation alkenal alkenol catalyst; **rhodium** phosphine ligand hydroformylation catalyst; pentenal manuf hydroformylation butadiene

IT **Aldehydes, preparation**
RL: IMF (Industrial manufacture); PREP (Preparation)
(C5; selective manufacture of **alkenals** and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **Aldehydes, preparation**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(**alkenals**; selective manufacture of **alkenals** and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **Alcohols**, preparation
RL: IMF (Industrial manufacture); PREP (Preparation)
(alkenols; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **Dialdehydes**
RL: BYP (Byproduct); PREP (Preparation)

(formation of; in selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT Hydroformylation catalysts
(selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)
(selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses 1038-95-5, Tris(p-tolyl)phosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 6372-40-3, Isopropyldiphenylphosphine 6737-42-4 **12150-46-8** 14874-82-9, **Rhodium** dicarbonyl acetylacetonate 32305-98-9 53111-20-9 61806-56-2, Phenylbis(cyanomethyl)phosphine **84680-96-6** 108793-33-5 121627-17-6 138776-88-2 138776-89-3 154813-98-6 198475-94-4
RL: CAT (Catalyst use); USES (Uses)
(catalyst; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **110-62-3P**, **Valeraldehyde** 629-11-8P, 1,6-Hexanediol 1072-21-5P, **Adipaldehyde** 34067-76-0P, 6-Hydroxyhexanal
RL: BYP (Byproduct); PREP (Preparation)
(formation of; in selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **96-17-3P**, 2-**Methylbutyraldehyde** 25167-67-3P, Butene 100080-07-7P
RL: BYP (Byproduct); PREP (Preparation)
(formation of; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

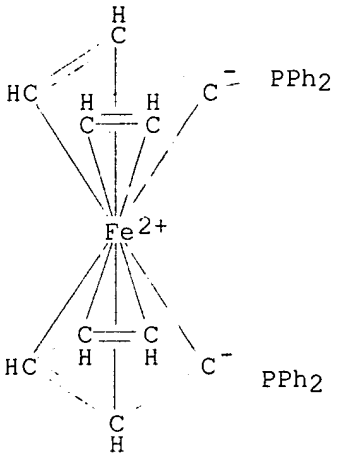
IT 106-99-0, Butadiene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroformylation of; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT 764-37-4DP, trans-3-Penten-1-ol, derivs. 764-37-4P, trans-3-Penten-1-ol 764-38-5DP, cis-3-Penten-1-ol, derivs. 764-38-5P, cis-3-Penten-1-ol 821-09-0DP, 4-Penten-1-ol, derivs. 821-09-0P, 4-Penten-1-ol 1576-86-9DP, cis-2-Pentenal, derivs. 1576-86-9P, cis-2-Pentenal 1576-87-0DP, trans-2-Pentenal, derivs. 1576-87-0P, trans-2-Pentenal 1576-95-0DP, cis-2-Penten-1-ol, derivs. 1576-95-0P, cis-2-Penten-1-ol 1576-96-1DP, trans-2-Penten-1-ol, derivs. 1576-96-1P, trans-2-Penten-1-ol 2100-17-6DP, 4-Pentenal, derivs. 2100-17-6P, 4-Pentenal 53448-06-9DP, cis-3-Pentenal, derivs. 53448-06-9P 58838-14-5DP, derivs. 58838-14-5P, trans-3-Pentenal
RL: IMF (Industrial manufacture); PREP (Preparation)
(selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT 106-99-0D, Butadiene, derivs. 630-08-0, Carbon monoxide, reactions 1333-74-0, Hydrogen, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **12150-46-8** **84680-96-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

RN 12150-46-8 HCAPLUS
CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



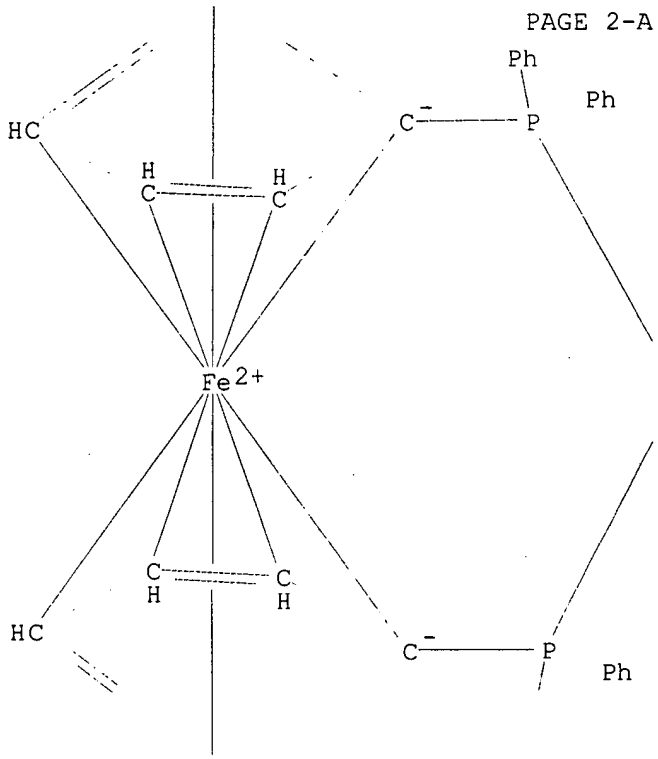
RN 84680-96-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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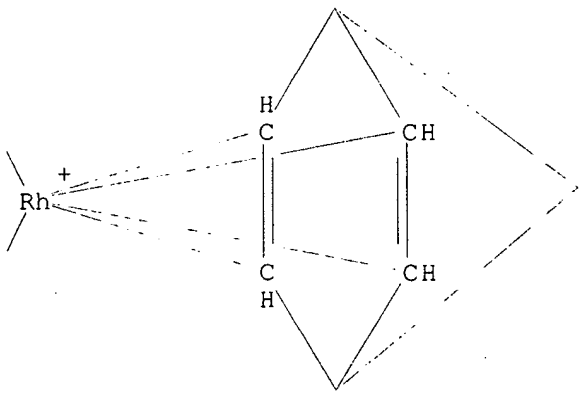
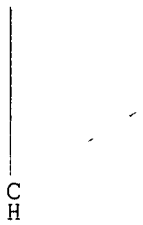
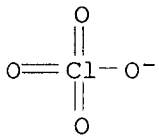




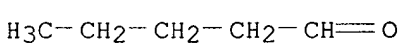
PAGE 3-A
Ph

CM 2

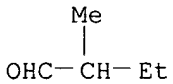
CRN 14797-73-0
CMF Cl O4



IT **110-62-3P, Valeraldehyde**
RL: BYP (Byproduct); PREP (Preparation)
(formation of; in selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
RN 110-62-3 HCAPLUS
CN Pentanal (9CI) (CA INDEX NAME)



IT **96-17-3P**, 2-**Methylbutyraldehyde**
RL: BYP (Byproduct); PREP (Preparation)
(formation of; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
RN 96-17-3 HCAPLUS
CN Butanal, 2-methyl- (9CI) (CA INDEX NAME)



L104 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:756952 HCAPLUS
DN 128:14353
ED Entered STN: 04 Dec 1997
TI Manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor
IN Briggs, John Robert; Packett, Diane Lee; Bryant, David Robert; Phillips, Ailene Gardner; Schreck, David James; Olson, Kurt Damar; Tjaden, Erick Bruce; Guram, Anil Sakharam; Eisenschmid, Thomas Carl; Bragham, Elaine Susan
PA Union Carbide Chemicals and Plastics Technology Corp., USA
SO PCT Int. Appl., 113 pp.
CODEN: PIXXD2

DT Patent
LA English
IC C07C045-49; C07C043-68; C07C029-16; C07C045-50; C07C047-19
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 35, 67
FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9740001	A1	19971030	WO 1997-US6881	19970423 <--
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	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9727421	A1	19971112	AU 1997-27421	19970423 <--
	EP 900187	A1	19990310	EP 1997-921364	19970423 <--
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	CN 1222904	A	19990714	CN 1997-195745	19970423 <--
	BR 9708863	A	19990803	BR 1997-8863	19970423 <--
	JP 2002500620	T2	20020108	JP 1997-538340	19970423 <--
	AT 223368	E	20020915	AT 1997-921364	19970423 <--
	ES 2178775	T3	20030101	ES 1997-921364	19970423 <--
	ES 2185006	T3	20030416	ES 1997-918801	19970423 <--
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	KR 2000011675	A	20000225	KR 1998-708639	19981023 <--
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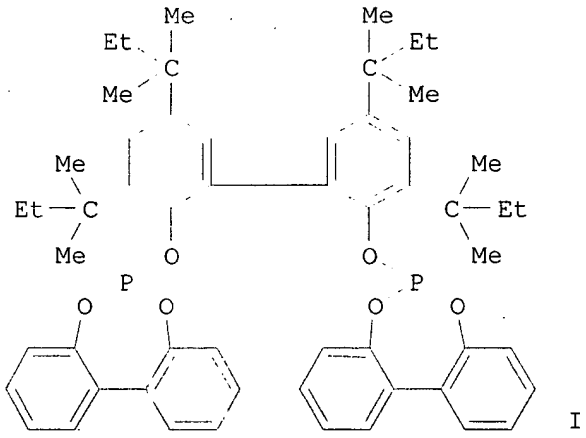
	US 1996-16259P	P	19960424 <--		
	US 1996-16263P	P	19960424 <--		
	US 1996-16378P	P	19960424 <--		
	US 1997-843340	A	19970415 <--		
	WO 1997-US6881	W	19970423 <--		

OS MARPAT 128:14353
GI



I

AB Substituted or unsubstituted **hydroxyaldehydes**, e.g., 6-hydroxyhexanals, are prepared by reductive hydroformylation of ≥1 (un)substituted alkadienes, e.g., butadiene, or pentenals in the presence of a reductive hydroformylation catalyst, e.g., a metal-organophosphorus

ligand complex catalyst, and hydroformylation of the unsatd. **alcs** . in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst. The (un)substituted **hydroxyaldehydes** can undergo further reaction(s) to afford desired derivs., e.g., ε-caprolactone (no data). Thus, liquid butadiene was charged to a reactor containing a THF solution of **rhodium** dicarbonyl acetylacetonate (200 ppm **Rh**) and 6,6'-[[3,3'5,5'-tetrakis(1,1-dimethylpropyl)[1,1'-biphenyl]-2,2'-diyl]bis(oxy)]bis-dibenzo[d,f][1,3,2]dioxaphosphepin (I) (12:1 ligand-**Rh** ratio), heated to 95° and pressurized to 500 psig with 1:1 CO-H2, giving, after 2 h, 95% butadiene conversion to 3-pentenals 75, 4-pentenal 3, 2-pentenals 5, **valeraldehyde** 7, branched **dialdehyde** 1, and **adipaldehyde** 9%.

ST **hydroxyaldehyde** manuf hydroformylation alkadiene pentenal **alc**; metal organophosphorus ligand hydroformylation catalyst; butadiene reductive hydroformylation catalyst **hydroxyaldehyde** manuf; **rhodium** dicarbonyl acetylacetonate hydroformylation catalyst; phosphine ligand hydroformylation catalyst

IT **Aldehydes, preparation**
RL: IMF (Industrial manufacture); PREP (Preparation)
(C5, preparation of; in manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or **unsatd.** **alcs**. and catalysts therefor)

IT **Dialdehydes**
RL: BYP (Byproduct); PREP (Preparation)
(branched, formation of; in manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

IT **Aldehydes, preparation**
RL: IMF (Industrial manufacture); PREP (Preparation)
(**hydroxy**; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or **unsatd.** **alcs**. and catalysts therefor)

IT Hydroformylation catalysts
(manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

IT **Alcohols**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(unsatd.; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

IT **96-17-3P**, 2-**Methylbutyraldehyde** **110-62-3P**, **Valeraldehyde** 764-39-6P, 2-Pentenal 1072-21-5P, **Adipaldehyde** 2100-17-6P, 4-Pentenal 5604-55-7P, 3-Pentenal 25167-67-3P, Butene 100080-07-7P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor)

IT 71-41-0DP, Pentan-1-ol, derivs. **110-62-3DP**, **Valeraldehyde**, derivs. **111-30-8DP**, 1,5-Pentanedial, derivs. 638-37-9DP, 1,4-Butanedial, derivs. 1072-21-5DP, 1,6-Hexanedial, derivs.
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

IT 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses

607-01-2, Ethyldiphenylphosphine 672-66-2 1038-95-5, Tris(p-tolyl)phosphine 1605-53-4, Diethylphenylphosphine 2234-97-1, Tripropylphosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 4731-53-7, Trioctylphosphine 6372-40-3, Isopropyldiphenylphosphine 6737-42-4 **12150-46-8** 14874-82-9, **Rhodium** dicarbonyl acetylacetonate 19262-01-2 32305-98-9 32376-20-8, tert-Butyldiethylphosphine 50420-43-4 53111-20-9 **84680-96-6** 108793-33-5 121627-17-6 138776-88-2 138776-89-3 154813-98-6 198475-94-4
RL: CAT (Catalyst use); USES (Uses)
(catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor)

IT 19584-30-6, **Tetrarhodium** dodecacarbonyl 76189-55-4 111982-81-1, 2,2'-(Bisdiphenylphosphinomethyl)-1,1'-biphenyl 154814-02-5 169254-16-4 198478-30-7 198478-33-0 198478-35-2
RL: CAT (Catalyst use); USES (Uses)
(catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of unsatd. **alcs**. and catalysts therefor)

IT 764-37-4P, trans-3-Penten-1-ol 60544-74-3P, 2-Pentenol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and reaction of; manufacture of **hydroxyaldehydes** by hydroformylation of unsatd. **alcs**. and catalysts therefor)

IT 71-41-0P, 1-Pentanol, preparation
RL: BYP (Byproduct); PREP (Preparation)
(formation in hydroformylation of cis-3-pentenol; manufacture of **hydroxyaldehydes** by hydroformylation of unsatd. **alcs**. and catalysts therefor)

IT 106-99-0D, Butadiene, derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes and catalysts therefor)

IT 106-99-0, Butadiene, reactions 630-08-0, Carbon monoxide, reactions 1333-74-0, Hydrogen, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor)

IT 4221-03-8DP, 5-Hydroxypentanal, derivs. 4221-03-8P, 5-Hydroxypentanal 25714-71-0DP, 4-Hydroxybutanal, derivs. 25714-71-0P, 4-Hydroxybutanal 34067-76-0DP, 6-Hydroxyhexanal, derivs. 34067-76-0P, 6-Hydroxyhexanal
RL: IMF (Industrial manufacture); PREP (Preparation)
(manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

IT 31424-04-1D, Pentenal, derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

IT 764-38-5, cis-3-Pentenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of **hydroxyaldehydes** by hydroformylation of unsatd. **alcs**. and catalysts therefor)

IT 156619-80-6P, Penten-1-ol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

IT 156619-80-6D, Penten-1-ol, derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and reaction of; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**.

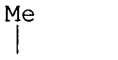
and catalysts therefor)

IT 821-09-0P, 4-Pentenol 1576-95-0P, cis-2-Penten-1-ol 1576-96-1P, trans-2-Penten-1-ol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of; manufacture of **hydroxyaldehydes** by hydroformylation of unsatd. **alcs**. and catalysts therefor)

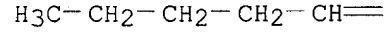
IT 695-06-7P 18545-19-2P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of; manufacture of **hydroxyaldehydes** by hydroformylation of unsatd. **alcs**. and catalysts therefor)

IT **96-17-3P**, 2-**Methylbutyraldehyde 110-62-3P**, **Valeraldehyde**
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor)

RN 96-17-3 HCAPLUS
CN Butanal, 2-methyl- (9CI) (CA INDEX NAME)

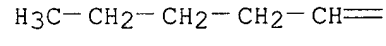


RN 110-62-3 HCAPLUS
CN Pentanal (9CI) (CA INDEX NAME)

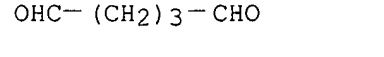


IT **110-62-3DP**, **Valeraldehyde**, derivs. **111-30-8DP**, 1,5-Pentanedial, derivs.
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs**. and catalysts therefor)

RN 110-62-3 HCAPLUS
CN Pentanal (9CI) (CA INDEX NAME)

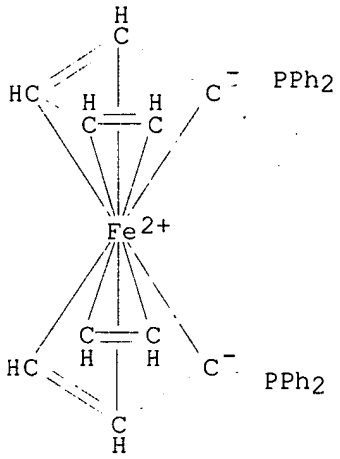


RN 111-30-8 HCAPLUS
CN Pentanedial (9CI) (CA INDEX NAME)



IT **12150-46-8 84680-96-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor)

RN 12150-46-8 HCAPLUS
CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



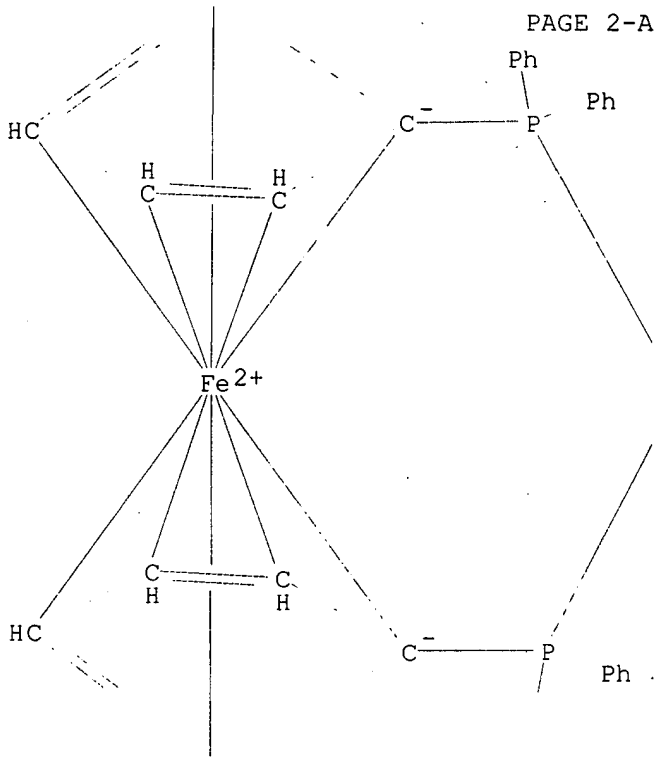
RN 84680-96-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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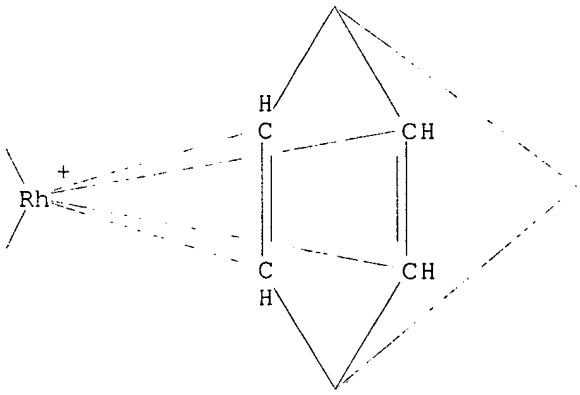

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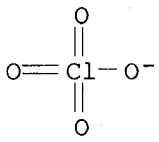
CRN 14797-73-0
CMF Cl O4



L104 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:740058 HCAPLUS
DN 128:13065
ED Entered STN: 24 Nov 1997
TI Preparation of alkenols by reductive hydroformylation of alkadienes.
IN Packett, Diane Lee; Briggs, John Robert; Bryant, David Robert; Phillips, Ailene Gardner; Schreck, David James; Guram, Anil Sakharam; Olson, Kurt Dawar; Eisenschmid, Thomas Carl; Tjaden, Erik Bruce
PA Union Carbide Chemicals and Plastics Technology Corp., USA
SO PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DT Patent
LA English
IC C07C029-16; C07C031-20
CC 23-7 (Aliphatic Compounds)
FAN.CNT 7

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9739996	A1	19971030	WO 1997-US6852	19970423 <--
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	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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	US 2002007096	A1	20020117	US 1997-842666	19970415 <--
	AU 9728093	A1	19971112	AU 1997-28093	19970423 <--
	US 6369283	B1	20020409	US 2000-704411	20001102 <--
PRAI	US 1996-15947P	P	19960424 <--		
	US 1996-16287P	P	19960424 <--		
	US 1997-842666	A	19970415 <--		
	US 1997-843381	A3	19970415 <--		
	WO 1997-US6852	W	19970423 <--		

OS CASREACT 128:13065; MARPAT 128:13065
AB Catalytic reductive hydroformylation of ≥1 alkadiene selectively produces ≥1 (substituted) alkenol. Thus, a solution of

rhodium dicarbonyl acetylacetonate and trioctylphosphine in octanol was pressurized with butadiene and 600 psi CO/200 psi H2 and heated at 80° to give 98% butadiene conversion and 88% selectivity for 3- and 4-pentenols.

ST butadiene reductive hydroformylation; alkenol prepn; pentenol prepn; alkadiene reductive hydroformylation

IT **Alcohols**, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(alkenols; preparation of alkenols by reductive hydroformylation of alkadienes)

IT Hydroformylation catalysts
(**dicarbonylacetylacetonatorhodium**(I) with phosphine ligands for reductive hydroformylation; preparation of alkenols by reductive hydroformylation of alkadienes)

IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of alkenols by reductive hydroformylation of alkadienes)

IT Hydroformylation
(reductive hydroformylation; preparation of alkenols by reductive hydroformylation of alkadienes)

IT 71-41-0P, 1-Pentanol, preparation **110-62-3P**, **Valeraldehyde** 1576-86-9DP, cis-2-Pentenal, substituted 1576-86-9P, cis-2-Pentenal 1576-87-0DP, trans-2-Pentenal, substituted 1576-87-0P, trans-2-Pentenal 2100-17-6DP, 4-Pentenal, substituted 2100-17-6P, 4-Pentenal 53448-06-9DP, cis-3-Pentenal, substituted 53448-06-9P, cis-3-Pentenal 58838-14-5DP, substituted 58838-14-5P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of alkenols by reductive hydroformylation of alkadienes)

IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses 607-01-2, Ethyldiphenylphosphine 1038-95-5, Tris(p-tolyl)phosphine 1605-53-4, Diethylphenylphosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 4706-17-6, Tris(3-hydroxypropyl)phosphine 4731-53-7, Trioctylphosphine 6372-40-3, Isopropyldiphenylphosphine 6737-42-4 10210-68-1, Dicobalt octacarbonyl **12150-46-8** 14874-82-9, **Rhodium** dicarbonylacetylacetonate 17005-57-1 19262-01-2 32305-98-9D, **rhodium** complex 32376-20-8, tert-Butyldiethylphosphine 50420-43-4 53111-20-9 60576-58-1 61806-56-2 **84680-96-6** 108793-33-5 121627-17-6 138776-88-2 138776-89-3 154813-98-6 198475-94-4
RL: CAT (Catalyst use); USES (Uses)
(preparation of alkenols by reductive hydroformylation of alkadienes)

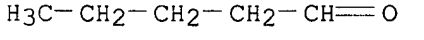
IT 764-37-4DP, trans-3-Penten-1-ol, substituted 764-37-4P, trans-3-Penten-1-ol 764-38-5DP, cis-3-Penten-1-ol, substituted 764-38-5P, cis-3-Penten-1-ol 821-09-0DP, 4-Penten-1-ol, substituted 821-09-0P, 4-Pentenol 1576-95-0DP, cis-2-Penten-1-ol, substituted 1576-95-0P, cis-2-Penten-1-ol 1576-96-1DP, trans-2-Penten-1-ol, substituted 1576-96-1P, trans-2-Penten-1-ol 77035-93-9P, 3-Pentenol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of alkenols by reductive hydroformylation of alkadienes)

IT 106-99-0, Butadiene, reactions 106-99-0D, Butadiene, substituted
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of alkenols by reductive hydroformylation of alkadienes)

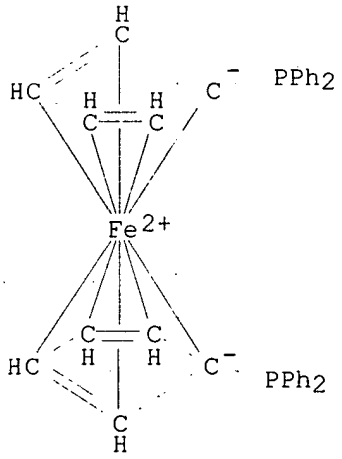
IT **110-62-3P**, **Valeraldehyde**
RL: BYP (Byproduct); PREP (Preparation)
(preparation of alkenols by reductive hydroformylation of alkadienes)

RN 110-62-3 HCAPLUS

CN Pentanal (9CI) (CA INDEX NAME)



IT **12150-46-8 84680-96-6**
RL: CAT (Catalyst use); USES (Uses)
(preparation of alkenols by reductive hydroformylation of alkadienes)
RN 12150-46-8 HCAPLUS
CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



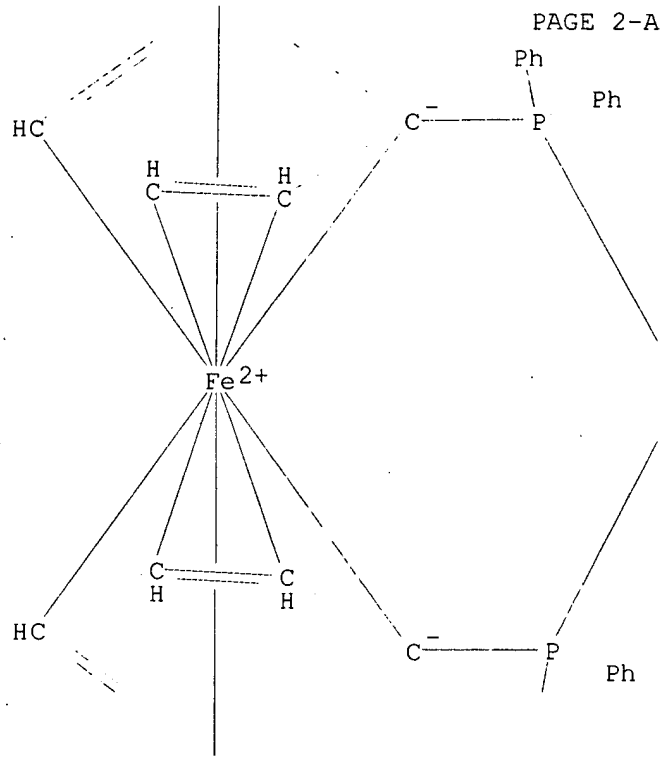
RN 84680-96-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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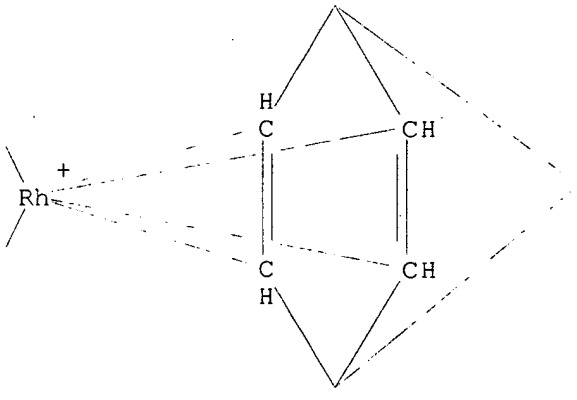

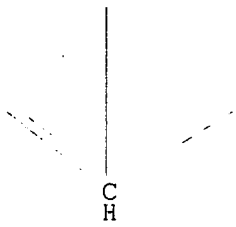

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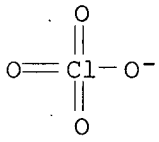
Ph

CM 2

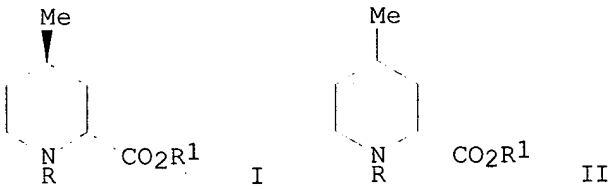
CRN 14797-73-0
CMF Cl O4



L104 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:733038 HCAPLUS
DN 127:358790
ED Entered STN: 21 Nov 1997
TI New method for preparing 2,4-trans-disubstituted piperidine derivatives
IN Grell, Wolfgang
PA Grell, Wolfgang, Germany
SO Ger. Offen., 30 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM C07D211-60
ICS C07B053-00
ICA C07D211-78; B01J031-24; B01J031-22
ICI C07M007-00; B01J023-46, B01J105-12
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 19616049	A1	19971030	DE 1996-19616049	19960423 <--
PRAI DE 1996-19616049		19960423 <--		

OS CASREACT 127:358790; MARPAT 127:358790
GI



AB Piperidines I [R = H, protective group; R1 = H, alkyl, protective group] were prepared by **hydrogenation** of tetrahydropyridines II [R =

protective group; R1 = alkyl, protective group] in presence of a **Rh** or Ru catalyst. Thus, PhCHMeN:CHCO2Et was cyclized with isoprene to give II [R = CHMePh, R1 = Et] which was **hydrogenated** over **rhodium**(I) [1,4-bis(diphenylphosphino)butane]-1c,5c-cyclooctadiene tetrafluoroborate followed by hydrogenolysis over Pd-C to give (2R,4R)-I [R = H, R1 = Et] with 93.6% de.

ST tetrahydropyridine stereoselective **hydrogenation** catalysts; piperidine disubstituted stereoselective prepn

IT **Hydrogenation catalysts**
(stereoselective; preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 7440-05-3, Palladium, uses 7440-16-6, **Rhodium**, uses 12122-73-5 12257-42-0 12279-09-3 14694-95-2, Tris(triphenylphosphine)**rhodium** chloride 15529-49-4 32761-50-5 32799-32-9 32965-49-4 35138-22-8 60576-58-1 62827-87-6 65012-74-0 79255-71-3 **84680-96-6** 126420-28-8 128363-26-8 130004-33-0 145926-28-9 198641-64-4
RL: CAT (Catalyst use); USES (Uses)
(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 78-79-5, reactions 100-46-9, Benzylamine, reactions **924-44-7**, Ethyl glyoxylate 2627-86-3, (S)-1-Phenylethylamine 35823-28-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 37662-06-9P 127897-25-0P 139334-63-7P 145774-82-9P 198641-56-4P 198641-60-0P 198641-62-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 74892-82-3P 78306-52-2P 79199-61-4P 139359-60-7P 145774-81-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT **84680-96-6**
RL: CAT (Catalyst use); USES (Uses)
(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

RN 84680-96-6 HCAPLUS

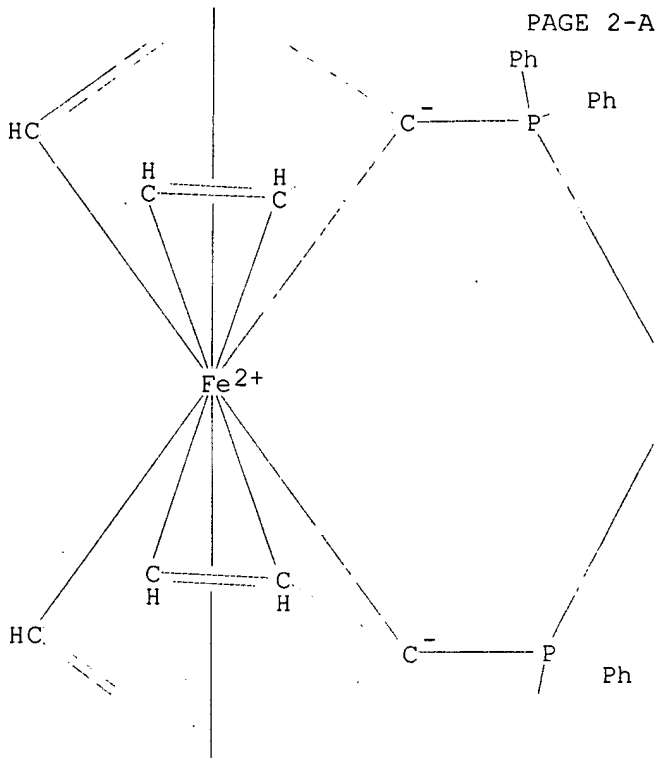
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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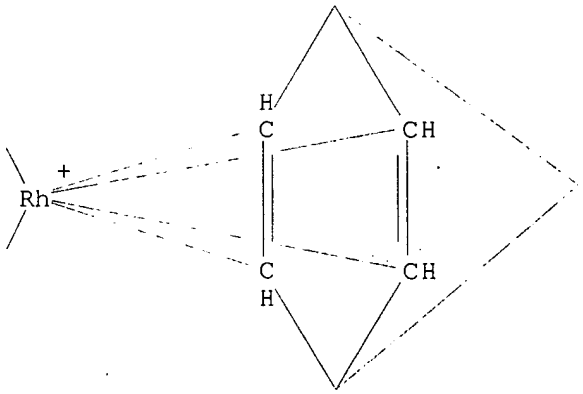
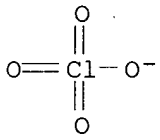


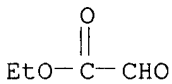
PAGE 3-A
Ph

CM 2

CRN 14797-73-0
CMF Cl O4



IT **924-44-7**, Ethyl glyoxylate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)
RN 924-44-7 HCAPLUS
CN Acetic acid, oxo-, ethyl ester (9CI) (CA INDEX NAME)



L104 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:57590 HCAPLUS
DN 126:144405
ED Entered STN: 27 Jan 1997
TI Group 9 metal 1,1'-bis(phosphino)ferrocene complexes: synthesis, structures, solution conformation and unusual reactivity
AU Avent, Anthony G.; Bedford, Robin B.; Chaloner, Penny A.; Dewa, Shaliza Z.; Hitchcock, Peter B.
CS School Chem. and Molecular Sciences, Univ. Sussex, Brighton, BN1 9QJ, UK
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (**1996**), (24), 4633-4638
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
AB The crystal structure of [Ir(cod)(L-L)]+ (3) [cod = cycloocta-1,5-diene, L-L = 1-(diisopropylphosphino)-1'-(diphenylphosphino)ferrocene] can be related to those of the analogous complexes with L-L = 1,1'-bis(diphenylphosphino)ferrocene (dppf) 1 and 1,1'-bis(diisopropylphosphino)ferrocene (disoppf), 2, all the complexes being readily synthesized from [Ir(cod)(py)2]+ (py = pyridine). An optimum diphosphine bite angle of .apprx.99° is maintained in all three

complexes by varying the twist of the ferrocene, which decreases with increasing steric profile of the phosphine, and by distortion of the geometry at the Ir atom away from square planar towards tetrahedral. The twist about the ferrocene moiety induces chirality at the Ir atom in all three complexes and the interchange of stereoisomers can be followed by variable-temperature 1H NMR spectroscopy. Application of the Eyring equation gave approx. values of ΔG.dbldag. for this process of 36.1 ± 0.2, 39.3 ± 0.2 and 34.3 ± 0.2 kJ mol-1 for 1-3 resp. The ligand disoppf also induces considerable distortion away from square-planar geometry in [**Rh**(nbd)(disoppf)][BF4] (4) {nbd = norbornadiene (bicyclo[2.2.1]hepta-2,5-diene)}, as found in a crystal structure determination, which may account for the unusual lability of the chelating diphosphine. This is demonstrated by its reactions with Ph2P(CH2)nPPh2 (n = 1 or 2) both of which give [**Rh**(L-L)2]+. More surprisingly, considering its lability in [**Rh**(nbd)(dppf)]+, dppf also readily displaced disoppf from 4, to give [**Rh**(nbd)(dppf)][BF4] (5). The nbd ligand in this complex is not displaced by reaction with an excess of dppf.

ST crystal structure iridium **rhodium** bisphosphinoferrocene diene; mol structure iridium **rhodium** bisphosphinoferrocene diene; kinetics conformational inversion iridium bisphosphinoferrocene diene; bisphosphinoferrocene iridium **rhodium** complex prepn structure; ferrocene bisphosphino iridium **rhodium** complex prepn; coordinative substitution **rhodium** bisphosphinoferrocene diene complex

IT Crystal structure
Molecular structure
(of iridium and **rhodium** diene bisphosphinoferrocene complexes)

IT Conformational transition
(of iridium bisphosphinoferrocene diene complexes)

IT Substitution reaction, coordinative
(of **rhodium** diene bisphosphinoferrocene complex)

IT 56678-60-5, (1,5-Cyclooctadiene)bis(pyridine)iridium(1+) hexafluorophosphate
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution reactions with bisphosphinoferrocenes)

IT **97239-80-0**, 1,1'-Bis(diisopropylphosphino)ferrocene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution reactions with iridium and **rhodium** diene complexes)

IT 36620-11-8, Bis(norbornadiene)**rhodium**(1+) tetrafluoroborate
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution with bis(diisopropylphosphino)ferrocene)

IT **97239-85-5**, 1-Diisopropylphosphino-1'-diphenylphosphinoferrocene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution with iridium COD pyridine complex)

IT 1663-45-2, 1,2-Bis(diphenylphosphino)ethane 2071-20-7, Bis(diphenylphosphino)methane **12150-46-8**, 1,1'-Bis(diphenylphosphino)ferrocene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution with **rhodium** bis(diisopropylphosphino)ferrocene diene complex)

IT 53450-77-4P, Bis(bis(diphenylphosphino)methane)**rhodium**(1+) 53450-79-6P, Bis(1,2-bis(diphenylphosphino)ethane)**rhodium**(1+) tetrafluoroborate **79790-98-0P**, (1,1'-Bis(diphenylphosphino)ferrocene)(norbornadiene)**rhodium**(1+) tetrafluoroborate
RL: SPN (Synthetic preparation); PREP (Preparation)
(formation by coordinative substitution with bis(diisopropylphosphino)ferrocene analog)

IT **151705-16-7**, (1,1'-Bis(diphenylphosphino)ferrocene)(1,5-

cyclooctadiene)iridium(1+) hexafluorophosphate
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(kinetics of conformational inversion and comparison to other bisphosphinoferrocene complexes)

IT **186692-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coordinative substitution reactions with diphosphines)

IT **186692-56-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

IT **167545-45-1P**, (1,1'-Bis(diisopropylphosphino)ferrocene)(1,5-cyclooctadiene)iridium(1+) tetraphenylborate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **186692-54-6P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation, crystal structure and kinetics of conformational inversion of)

IT **167545-42-8P**, (1,1'-Bis(diisopropylphosphino)ferrocene)(1,5-cyclooctadiene)iridium(1+) hexafluorophosphate
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation, metathesis and kinetics of conformational inversion of)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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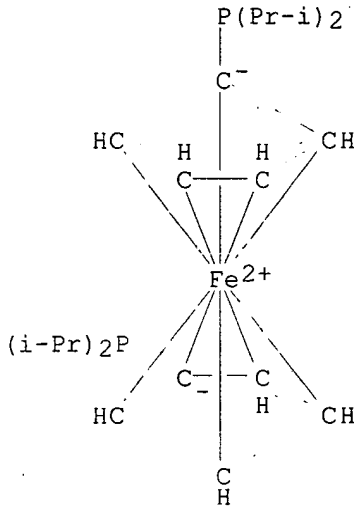
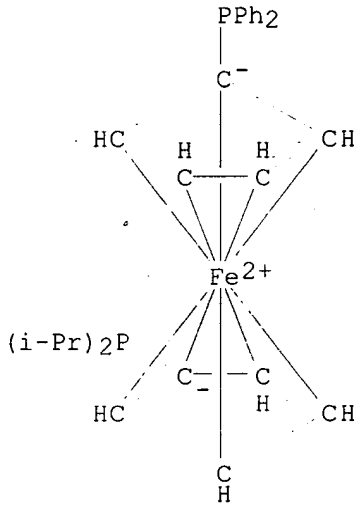
(23) Sheldrick, G; SHELXL 93 1993
(24) Sheldrick, G; SHELXS 86 1986
(25) Uson, R; Transition Met Chem 1979, V4, P55 HCAPLUS

IT **97239-80-0**, 1,1'-Bis(diisopropylphosphino)ferrocene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution reactions with iridium and **rhodium** diene complexes)

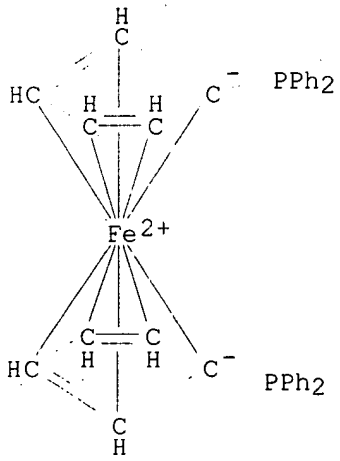
RN 97239-80-0 HCAPLUS
CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphino]- (9CI) (CA INDEX NAME)



IT **97239-85-5**, 1-Diisopropylphosphino-1'-diphenylphosphinoferrocene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution with iridium COD pyridine complex)
RN 97239-85-5 HCAPLUS
CN Ferrocene, 1-[bis(1-methylethyl)phosphino]-1'-(diphenylphosphino)- (9CI) (CA INDEX NAME)



IT **12150-46-8**, 1,1'-Bis(diphenylphosphino)ferrocene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution with **rhodium**
bis(diisopropylphosphino)ferrocene diene complex)
RN 12150-46-8 HCAPLUS
CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



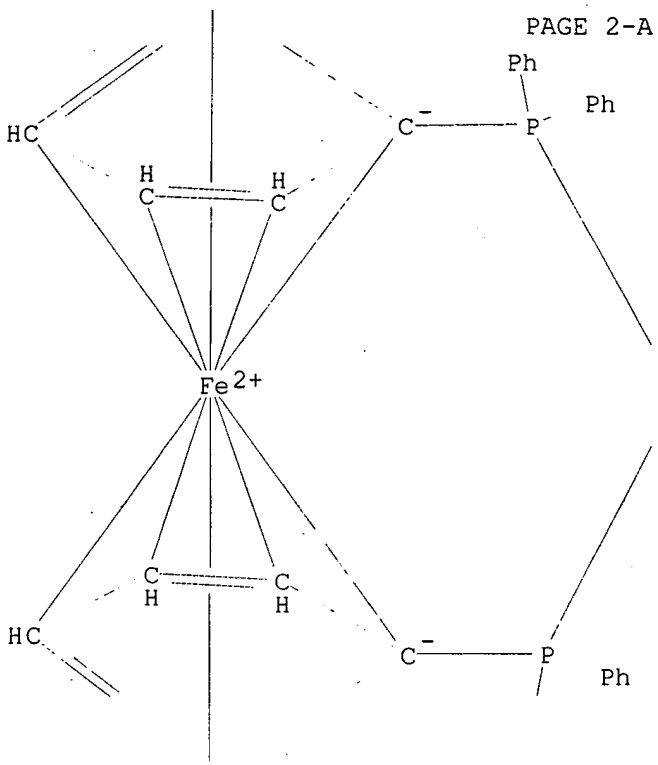
IT **79790-98-0P**, (1,1'-Bis(diphenylphosphino)ferrocene)(norbornadiene)**rhodium**(1+) tetrafluoroborate
RL: SPN (Synthetic preparation); PREP (Preparation)
(formation by coordinative substitution with bis(diisopropylphosphino)ferrocene analog)
RN 79790-98-0 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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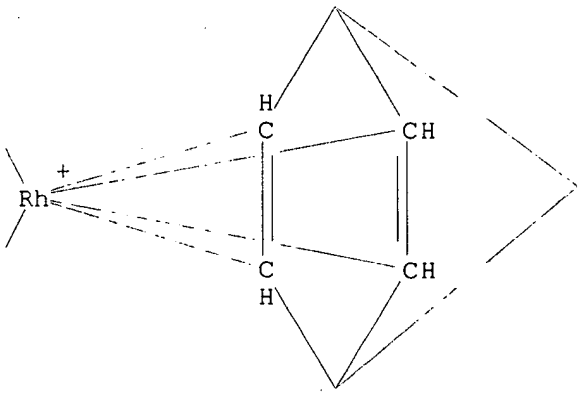

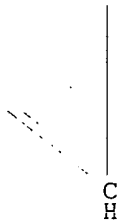

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Ph

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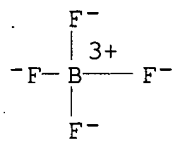
CRN 14874-70-5
CMF B F4
CCI CCS



IT **151705-16-7**, (1,1'-Bis(diphenylphosphino)ferrocene)(1,5-cyclooctadiene)iridium(1+) hexafluorophosphate
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(kinetics of conformational inversion and comparison to other bisphosphinoferrocene complexes)

RN 151705-16-7 HCAPLUS
CN Iridium(1+), [1,1'-bis(diphenylphosphino-κP)ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

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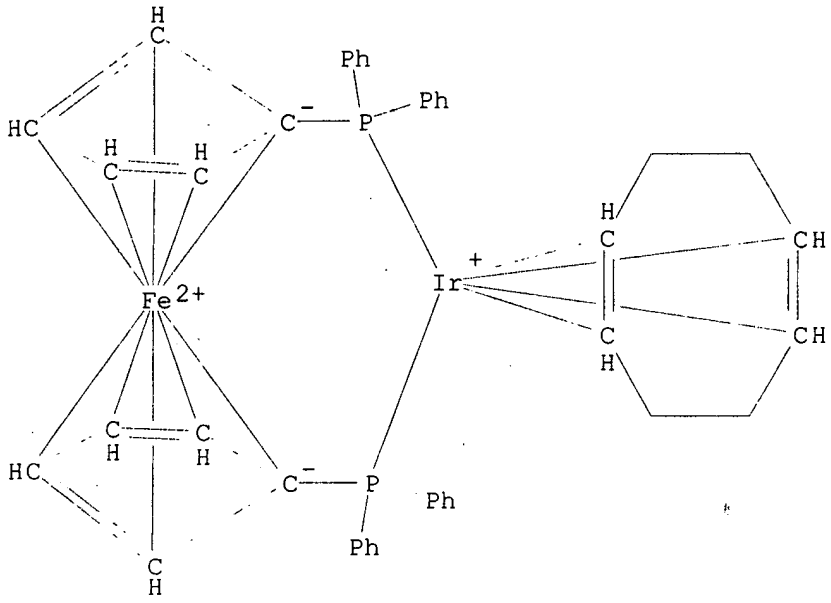
CCI CCS



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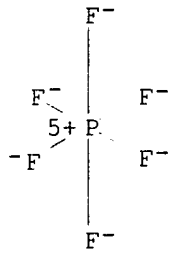
CRN 16919-18-9
CMF F6 P
CCI CCS



IT **186692-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coordinative substitution reactions with diphosphines)
RN 186692-55-7 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 96144-62-6
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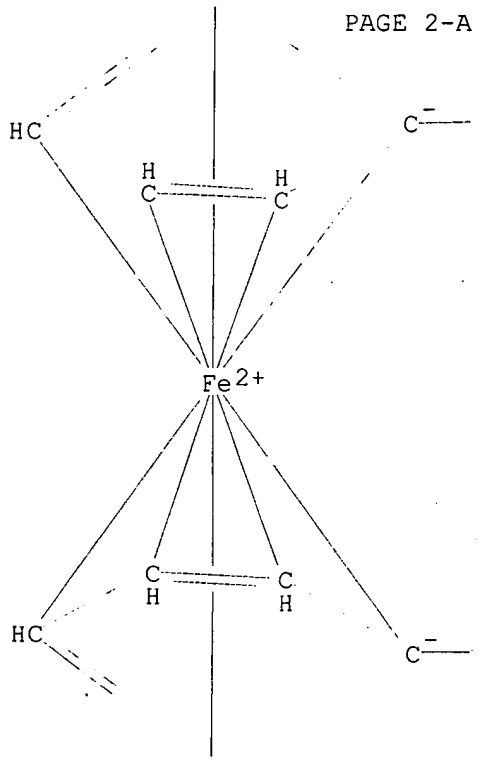
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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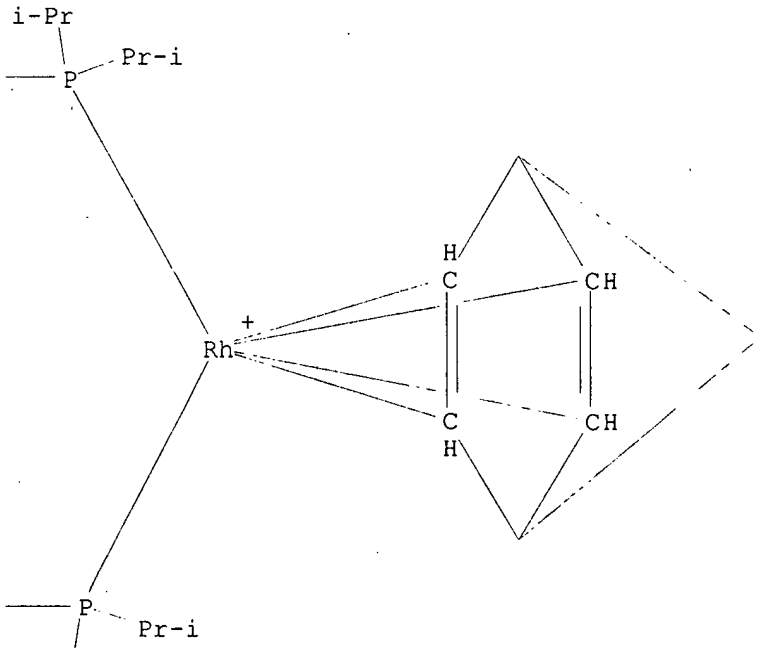


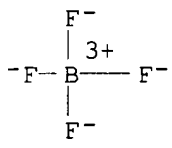
PAGE 3-A

PAGE 3-B

i-Pr

CM 2

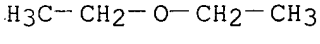
CRN 14874-70-5
CMF B F4
CCI CCS



IT **186692-56-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
RN 186692-56-8 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene]-, tetrafluoroborate(1-), compd. with 1,1'-oxybis[ethane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 60-29-7
CMF C4 H10 O



CM 2

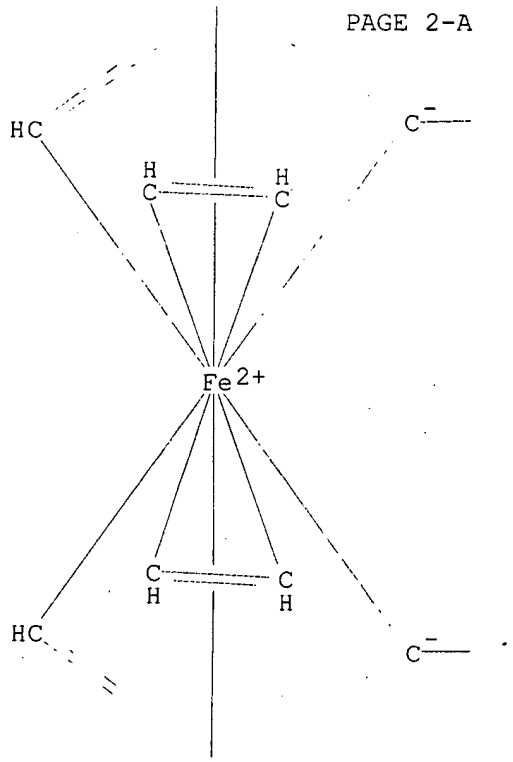
CRN 186692-55-7
CMF C29 H44 Fe P2 Rh . B F4

CM 3

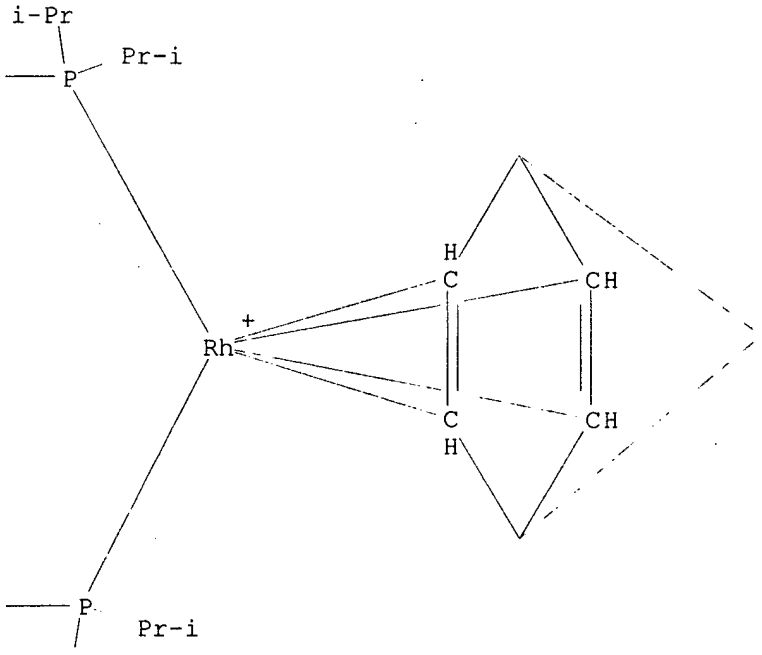
CRN 96144-62-6
CMF C29 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



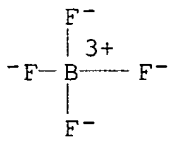
PAGE 3-A

PAGE 3-B

i-Pr

CM 4

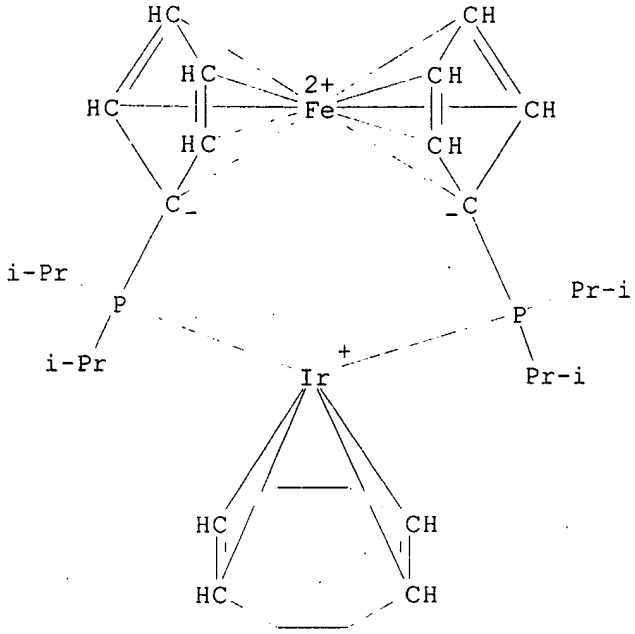
CRN 14874-70-5
CMF B F4
CCI CCS



IT **167545-45-1P**, (1,1'-Bis(diisopropylphosphino)ferrocene)(1,5-cyclooctadiene)iridium(1+) tetraphenylborate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 167545-45-1 HCAPLUS
CN Iridium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

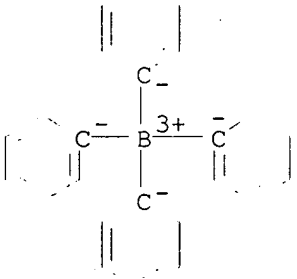
CM 1

CRN 167545-41-7
CMF C30 H48 Fe Ir P2
CCI CCS



CM 2

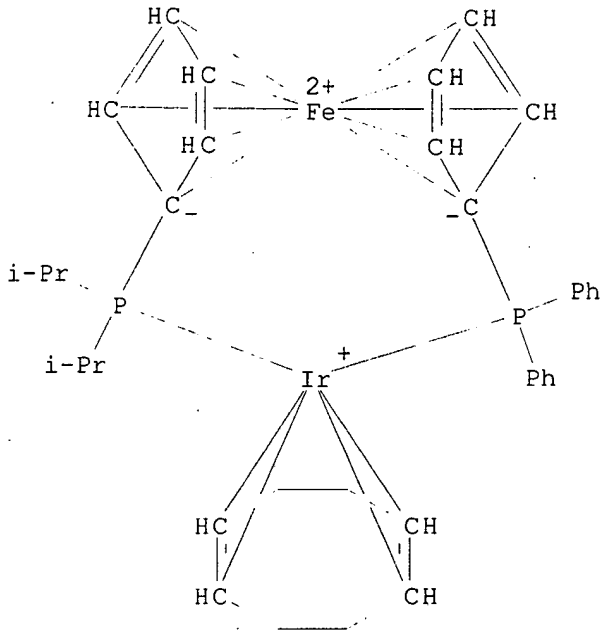
CRN 4358-26-3
CMF C24 H20 B
CCI CCS



IT **186692-54-6P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation, crystal structure and kinetics of conformational inversion of)
RN 186692-54-6 HCAPLUS
CN Iridium(1+), [1-[bis(1-methylethyl)phosphino-κP]-1'-(diphenylphosphino-κP)ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

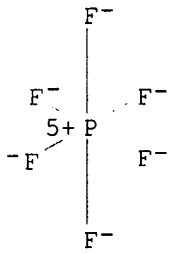
CM 1

CRN 186692-53-5
CMF C36 H44 Fe Ir P2
CCI CCS



CM 2

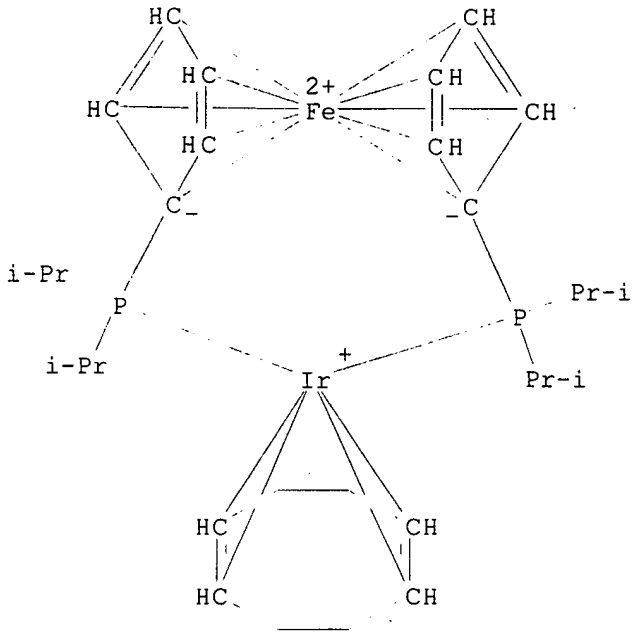
CRN 16919-18-9
CMF F6 P
CCI CCS



IT **167545-42-8P,** (1,1'-Bis(diisopropylphosphino)ferrocene)(1,5-cyclooctadiene)iridium(1+) hexafluorophosphate
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation, metathesis and kinetics of conformational inversion of)
RN 167545-42-8 HCAPLUS
CN Iridium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

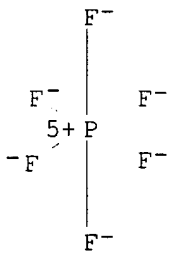
CM 1

CRN 167545-41-7
CMF C30 H48 Fe Ir P2
CCI CCS



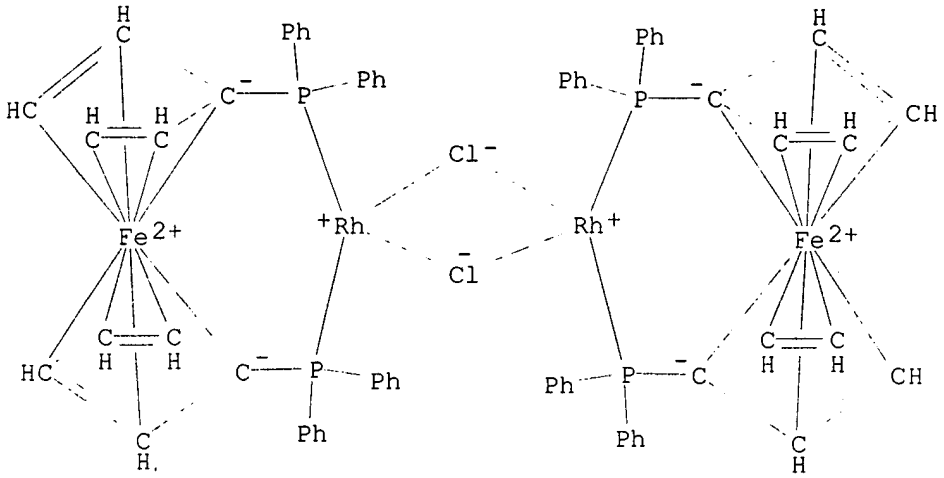
CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS



L104 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:1004413 HCAPLUS
DN 124:116619
ED Entered STN: 26 Dec 1995
TI Catalytic cyclization of some alkynes by rhodium and iridium complexes of ferrocene-containing ligands
AU Kim, Tae-Jeong; Kim, So-Hoon; Shim, Sang-Chul; Jeong, Jong-Hwa
CS Dep. of Industrial Chemistry, Kyungpook National Univ., Taegu, 702-701, S. Korea
SO Bulletin of the Korean Chemical Society (**1995**), 16(11), 1126-8
CODEN: BKCSDE; ISSN: 0253-2964
PB Korean Chemical Society
DT Journal
LA English

CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 29, 75
OS CASREACT 124:116619
AB The lactonization of 4-pentynoic acid and the cocyclotrimerization of N-benzylpropargylamine with PhC.tplbond.CH, both reaction catalyzed by Rh and Ir complexes with ferrocenylphosphines and -imines, were studied. [(COD)Ir(PPFA)]ClO4 (PPFA = 2-diphenylphosphino-1-(N,N-dimethylaminoethyl)ferrocene) was prepared and its crystal structure determined
ST crystal structure iridium aminoethylphosphinoferrocene; aminoethylphosphinoferrocene iridium prepn structure; cyclization catalyst iridium rhodium phosphinoferrocene alkyne
IT Alkynes
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic cyclization in presence of iridium and rhodium phosphinoferrocene complexes)
IT Ring closure catalysts
(iridium and rhodium phosphinoferrocene complexes for alkynes)
IT 536-74-3, Phenylacetylene 1197-51-9 6089-09-4, 4-Pentynoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic cyclization in presence of iridium and rhodium phosphinoferrocene complexes)
IT 91159-10-3 112947-51-0 **125939-72-2** 173101-24-1 173101-26-3 173101-28-5 173967-26-5
RL: CAT (Catalyst use); USES (Uses)
(cyclization catalysts for alkynes)
IT 12112-67-3, Dichlorobis(cyclooctadiene)diiridium 105088-01-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of iridium cyclooctadiene aminoethylphosphinoferrocene complex)
IT 173101-31-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
IT 173101-30-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)
IT 10008-73-8P 173101-22-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation by catalytic cyclization of alkynes in presence of iridium and rhodium phosphinoferrocene complexes)
IT **125939-72-2**
RL: CAT (Catalyst use); USES (Uses)
(cyclization catalysts for alkynes)
RN 125939-72-2 HCAPLUS
CN Rhodium, bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di-μ-chlorodi- (9CI) (CA INDEX NAME)



L104 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:578803 HCAPLUS
DN 121:178803
ED Entered STN: 15 Oct 1994
TI Efficient **rhodium**-catalyzed **hydrogenation** of **aldehydes** and ketones
AU **Burk, Mark J.**; Harper, T. Gregory P.; Lee, Jeffrey R.; Kalberg, Christopher
CS Dep. Chem., Duke Univ., Durham, NC, 27706, USA
SO Tetrahedron Letters (**1994**), 35(28), 4963-6
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
OS CASREACT 121:178803
AB A cationic **rhodium**(I) catalyst bearing the air-stable and crystalline diphosphine 1,1'-bis(diisopropylphosphino)ferrocene allows the **hydrogenation** of **aldehydes** and ketones under mild conditions.
ST **rhodium** ferrocene catalyst **hydrogenation** carbonyl; **aldehyde hydrogenation rhodium** catalyst; ketone **hydrogenation rhodium** catalyst
IT **Aldehydes, reactions**
Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, **rhodium** ferrocene complex as catalyst for)
IT **Hydrogenation catalysts**
(**rhodium** ferrocene complex, for **aldehydes** and ketones)
IT **97239-80-0**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing bis(cyclooctadiene)**rhodium** triflate, for **hydrogenation** of **aldehydes** and ketones)
IT 99326-34-8
RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing bis(diisopropylphosphino)ferrocene, for **hydrogenation** of **aldehydes** and ketones)
IT **157772-66-2**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for **hydrogenation** of **aldehydes** and ketones)

IT **66-25-1**, Hexanal 78-93-3, 2-Butanone, reactions **98-01-1**, 2-**Furancarboxaldehyde**, reactions **98-03-3**, 2-**Thiophenecarboxaldehyde** 98-53-3 98-86-2, Acetophenone, reactions **100-52-7**, **Benzaldehyde**, reactions 108-94-1, Cyclohexanone, reactions 119-53-9, Benzoin 122-57-6, Benzalacetone 372-31-6 434-45-7, Trifluoroacetophenone 513-86-0 609-38-1, 2-Furancarboxamide **630-19-3**, **Pivalaldehyde** 1603-79-8, Ethyl oxophenylacetate 1694-31-1, tert-Butyl 3-oxobutanoate 3524-62-7 3891-59-6 7152-15-0, Pentanoic acid, 4-methyl-3-oxo-, ethyl ester 20201-24-5, Butanoic acid, 3-methyl-2-oxo-, ethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, **rhodium** ferrocene complex as catalyst for)

IT 2550-26-7P, 4-Phenyl-2-butanone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **hydrogenation** of, **rhodium** ferrocene complex as catalyst for)

IT 2344-70-9P, 4-Phenyl-2-butanol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 100-51-6P, Benzyl **alcohol**, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by **rhodium** complex-catalyzed **hydrogenation** of **benzaldehyde**)

IT 579-43-1P 655-48-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by **rhodium** complex-catalyzed **hydrogenation** of benzoin)

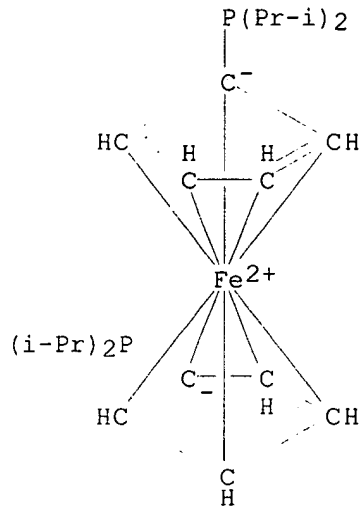
IT 5341-95-7P 6982-25-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by **rhodium** complex-catalyzed **hydrogenation** of hydroxybutanone)

IT 937-05-3P, Cyclohexanol, 4-(1,1-dimethylethyl)-, cis- 21862-63-5P, Cyclohexanol, 4-(1,1-dimethylethyl)-, trans-
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by **rhodium** complex-catalyzed **hydrogenation** of ketone)

IT **97239-80-0**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing bis(cyclooctadiene)**rhodium** triflate, for **hydrogenation** of **aldehydes** and ketones)

RN 97239-80-0 HCAPLUS

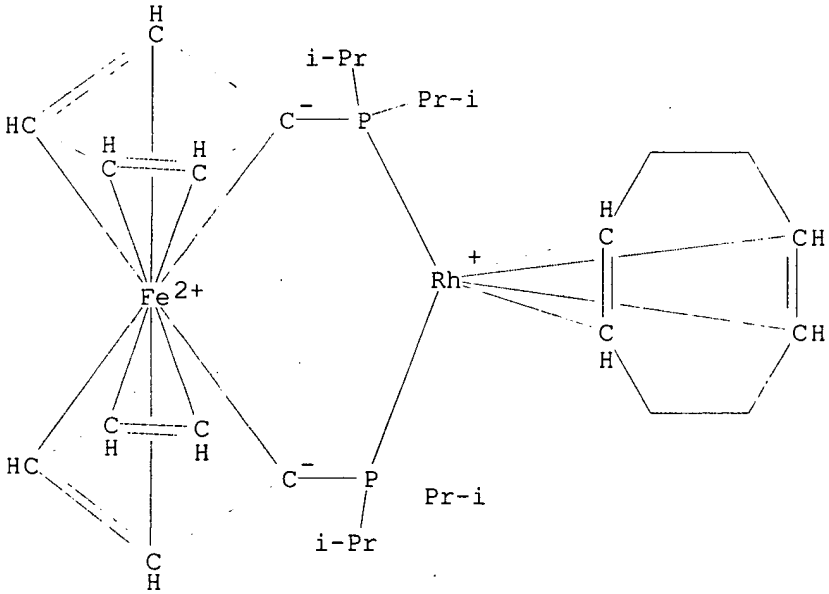
CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphino]- (9CI) (CA INDEX NAME)



IT **157772-66-2**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for **hydrogenation** of **aldehydes** and ketones)
RN 157772-66-2 HCAPLUS
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P'][(1,2,5,6-η)-1,5-cyclooctadiene]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

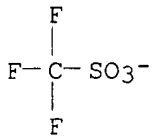
CM 1

CRN 157772-65-1
CMF C30 H48 Fe P2 Rh
CCI CCS

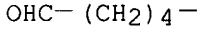


CM 2

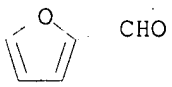
CRN 37181-39-8
CMF C F3 O3 S



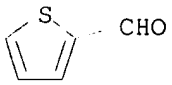
IT **66-25-1**, Hexanal **98-01-1**, 2-**Furancarboxaldehyde**, reactions **98-03-3**, 2-**Thiophenecarboxaldehyde** **100-52-7**, **Benzaldehyde**, reactions **630-19-3**, **Pivalaldehyde**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, **rhodium** ferrocene complex as catalyst for)
RN 66-25-1 HCAPLUS
CN Hexanal (8CI, 9CI) (CA INDEX NAME)



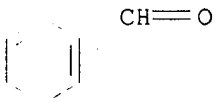
RN 98-01-1 HCAPLUS
CN 2-Furancarboxaldehyde (9CI) (CA INDEX NAME)



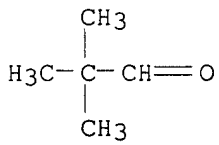
RN 98-03-3 HCAPLUS
CN 2-Thiophenecarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 100-52-7 HCAPLUS
CN Benzaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



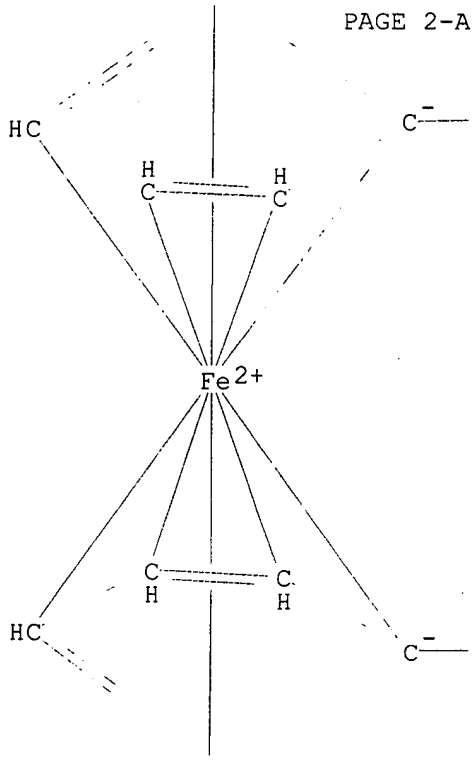
RN 630-19-3 HCAPLUS
CN Propanal, 2,2-dimethyl- (9CI) (CA INDEX NAME)



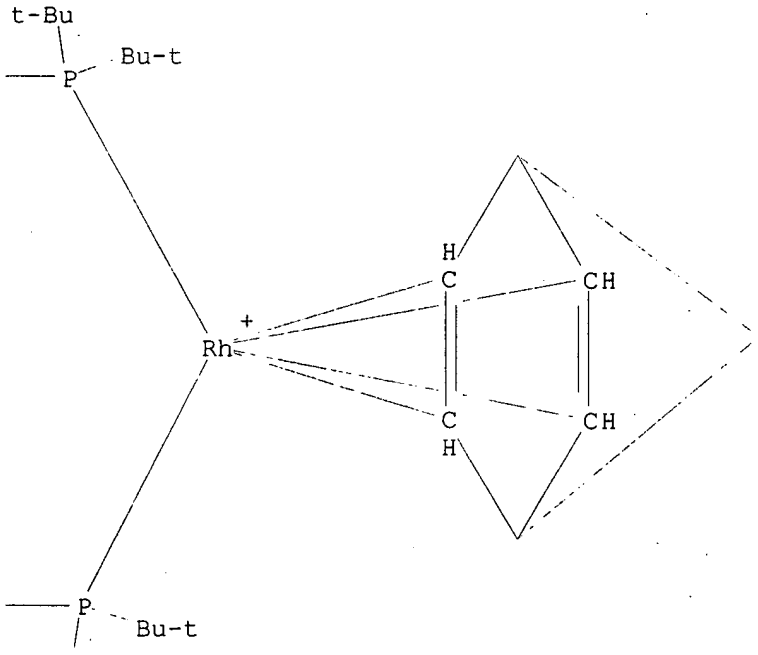
L104 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:603799 HCAPLUS
DN 113:203799
ED Entered STN: 23 Nov 1990
TI Synthesis and solution chemistry of metal hydrides from cationic **rhodium**(I) catalyst precursors [(L-L)**Rh**(NBD)]ClO4 (L-L = Fe(η5-C5H4PBu-tert2)2, Fe(η5-C5H4PPhBu-tert)2)
AU Kim, Tae Jeong
CS Dep. Ind. Chem., Kyungpook Natl. Univ., Taegu, 702-701, S. Korea
SO Bulletin of the Korean Chemical Society (**1990**), 11(2), 134-9
CODEN: BKCSDE; ISSN: 0253-2964
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 29, 77
AB The **hydrogenation** catalyst precursors [(L-L)**Rh**(NBD)]ClO4 (L-L = Fe(η5-C5H4P(CMe3)2)2, Fe(η5-C5H4PPhCMe3)2; NBD = norbornadiene) react with H2 (1 atm, 30°, MeOH) to yield [(L-L)HRh(μ-H)3RhH(L-L)]ClO4. These hydrido species are fluxional, and variable temperature NMR studies show the existence of a number of equilibrium involving both fluxional and nonfluxional species. The synthesis, solution structures, and fluxional behaviors of these hydrides are described.
ST fluxionality **rhodium** hydrido ferrocenylphosphine dinuclear; phosphine ferrocenyl **rhodium** hydrido dinuclear
IT Fluxional rearrangement
(of **rhodium** hydrido ferrocenylphosphine dinuclear complexes)
IT **84680-97-7 92284-06-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)
IT **92468-70-7P 130322-22-4P**
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation and fluxionality of)
IT **84680-97-7 92284-06-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)
RN 84680-97-7 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']- (9CI) (CA INDEX NAME)

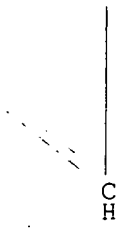
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B





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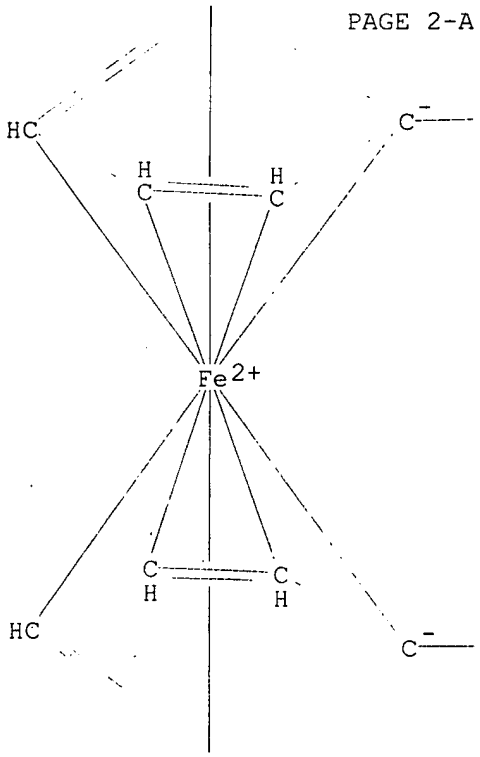
t-Bu

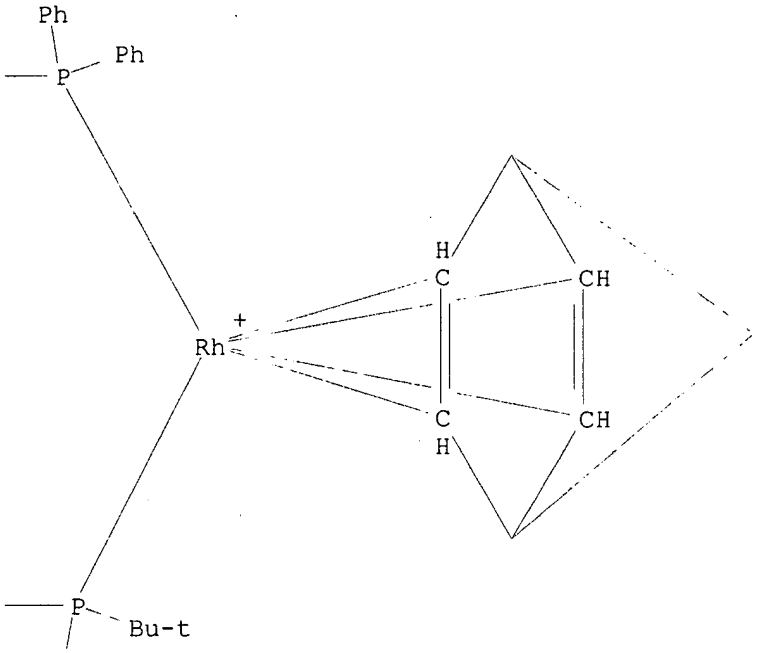
RN 92284-06-5 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']- (9CI) (CA INDEX NAME)

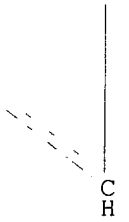
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B





PAGE 3-A

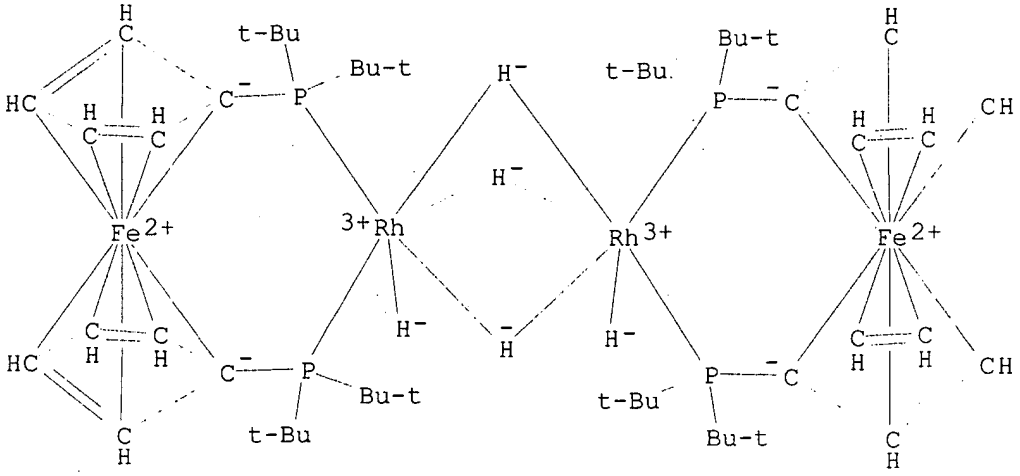
PAGE 3-B

t-Bu

IT **92468-70-7P 130322-22-4P**
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation and fluxionality of)
RN 92468-70-7 HCAPLUS
CN Rhodium(1+), bis[1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

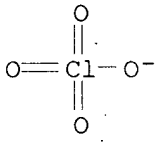
CM 1

CRN 92468-69-4
CMF C52 H93 Fe2 P4 Rh2
CCI CCS



CM 2

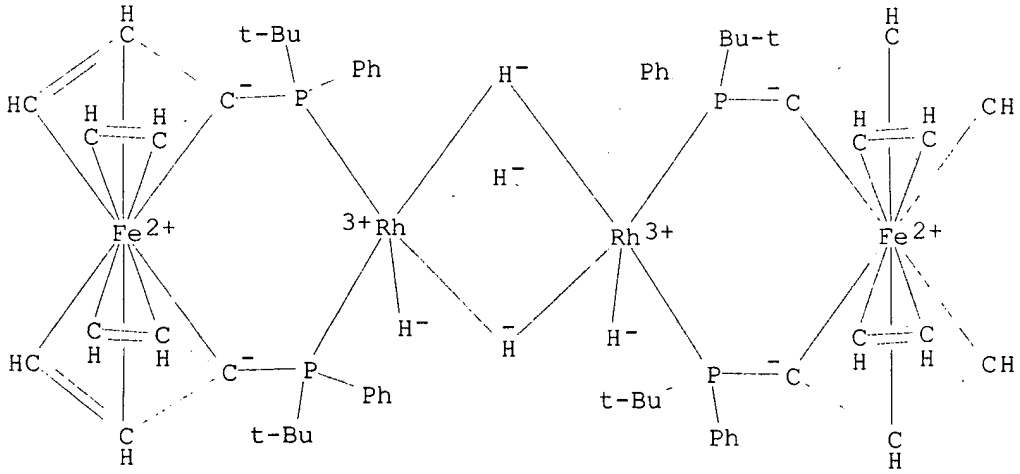
CRN 14797-73-0
CMF Cl O4



RN 130322-22-4 HCAPLUS
CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

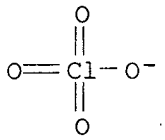
CM 1

CRN 130322-21-3
CMF C60 H77 Fe2 P4 Rh2
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4



L104 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:139478 HCAPLUS
DN 112:139478
ED Entered STN: 13 Apr 1990
TI **Rhodium**(I) complexes of 1,1'-bis(diphenylphosphino)ferrocene as efficient catalysts in regioselective hydrogenation of polynuclear heteroaromatic compounds
AU Kim, Tae Jeong; Lee, Kyu Chul
CS Dep. Ind. Chem., Kyungpook Natl. Univ., Taegu, 702-701, S. Korea
SO Bulletin of the Korean Chemical Society (**1989**), 10(3), 279-82
CODEN: BKCSDE; ISSN: 0253-2964
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 27
AB Two **rhodium**(I) complexes of the types [**Rh**(BPPF)(NBD)]ClO4 (I) and [**Rh**(BPPF)Cl]2 (II) (BPPF = 1,1'-bis(diphenylphosphino)ferrocene, NBD = norbornadiene) were prepared and investigated as catalysts for the regioselective hydrogenation of polynuclear heteroarom. N and S compds. such as quinoline, acridine, phenanthridine, 7,8-benzoquinoline, benzothiophene, isoquinoline, indole, pyridine, and thiophene. Both complexes I and II, except for the cases of indole and mononuclear heteroaroms. pyridine and thiophene, are very efficient in the selective reduction under quite mild hydrogenation conditions to give the corresponding saturated N and S heterocyclic analogs in fast conversion rates and in excellent yields. Relative rate studies revealed that the reduction depends significantly on the steric and electronic effects of the substrates. Of the two complexes, the dimeric species II gives faster reaction rates in all cases studied.
ST phenylphosphinoferrocene **rhodium** complex regioselective hydrogenation catalyst; heterocyclic nitrogen sulfur hydrogenation catalyst; kinetics hydrogenation nitrogen sulfur heterocycle
IT **Hydrogenation catalysts**
(bis(diphenylphosphino)ferrocene **rhodium** complexes, for nitrogen and sulfur heterocycles)
IT Regiochemistry
(of hydrogenation of nitrogen and sulfur heterocycles, **rhodium** complex-catalyzed)
IT Kinetics of hydrogenation
(of nitrogen and sulfur heterocyclic compds., **rhodium** -catalyzed)
IT Heterocyclic compounds
RL: RCT (Reactant); RACT (Reactant or reagent)
(nitrogen, regioselective hydrogenation of, **rhodium** catalysts for)
IT Heterocyclic compounds
RL: RCT (Reactant); RACT (Reactant or reagent)

(sulfur, regioselective hydrogenation of, **rhodium** catalysts for)

IT 110-02-1, Thiophene 110-86-1, Pyridine, reactions 120-72-9, 1H-Indole, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted hydrogenation of, **rhodium**-catalyzed)

IT **84680-96-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for regioselective hydrogenation of nitrogen and sulfur heterocycles)

IT 7727-37-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(heterocyclic compounds, nitrogen, regioselective hydrogenation of, **rhodium** catalysts for)

IT 7704-34-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(heterocyclic compounds, sulfur, regioselective hydrogenation of, **rhodium** catalysts for)

IT 91-22-5, Quinoline, reactions 95-15-8, Benzothiophene 119-65-3, Isoquinoline 229-87-8, Phenanthridine 230-27-3, 7,8-Benzoquinoline 260-94-6, Acridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of, (diphenylphosphino)**ferrocenerhodium** complex catalysts for, regiochem. and kinetics of)

IT **125939-72-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation as hydrogenation catalyst, for nitrogen and sulfur heterocycles)

IT 91-21-4P 92-81-9P 635-46-1P 4565-32-6P 5223-80-3P 27799-79-7P **125916-39-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **12150-46-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction by, of norbornadiene **rhodium** complex)

IT 12257-42-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with bis(diphenylphosphino)ferrocene)

IT **84680-96-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for regioselective hydrogenation of nitrogen and sulfur heterocycles)

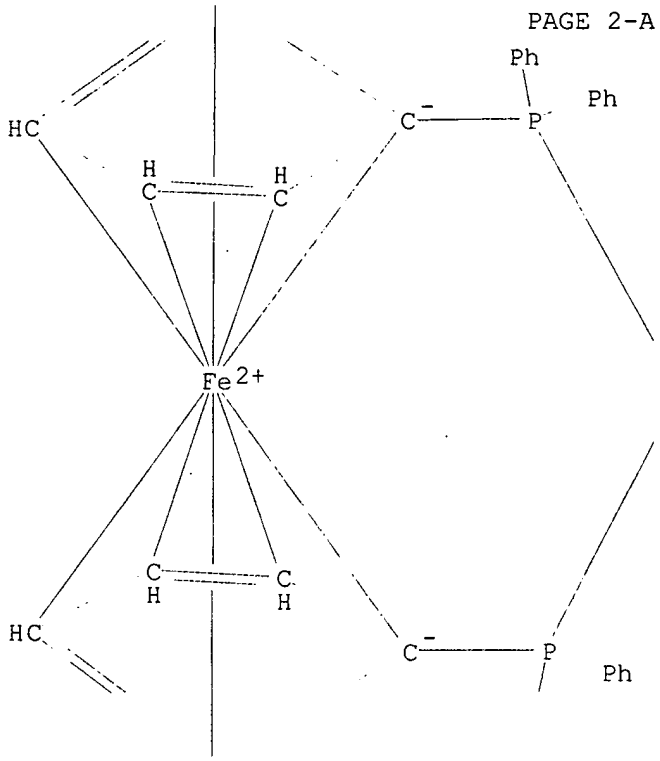
RN 84680-96-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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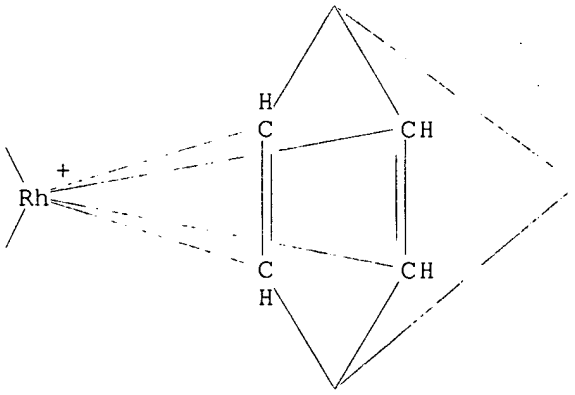
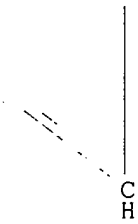
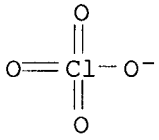




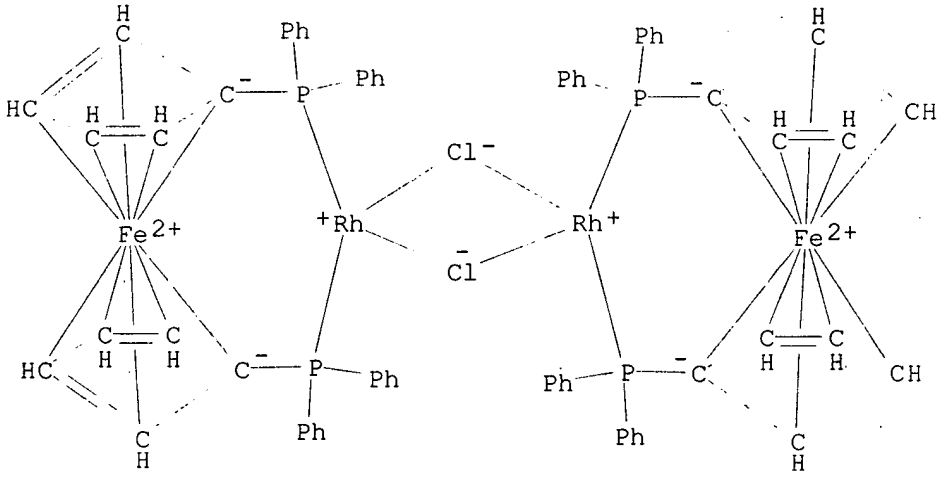
PAGE 3-A
Ph

CM 2

CRN 14797-73-0
CMF Cl O4



IT **125939-72-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation as hydrogenation catalyst, for nitrogen and sulfur heterocycles)
RN 125939-72-2 HCAPLUS
CN Rhodium, bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di-μ-chlorodi- (9CI) (CA INDEX NAME)

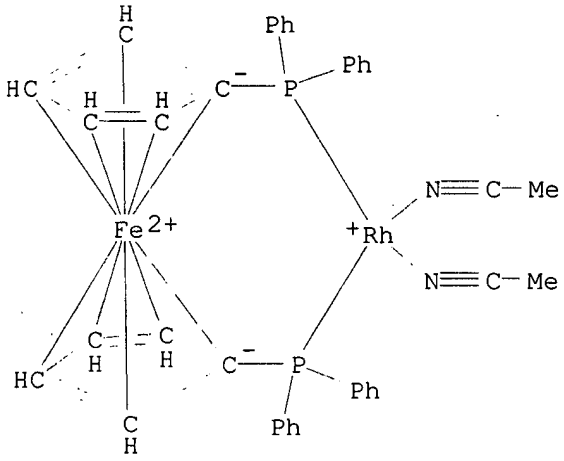


IT **125916-39-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 125916-39-4 HCAPLUS
CN Rhodium(1+), bis(acetonitrile)[1,1'-bis(diphenylphosphino)ferrocene-P,P']-, (SP-4-2)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

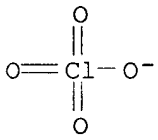
CRN 125916-38-3

CMF C38 H34 Fe N2 P2 Rh
CCI CCS

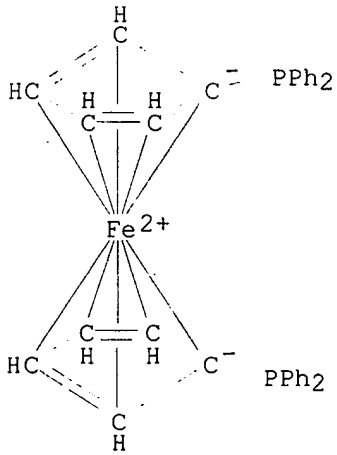


CM 2

CRN 14797-73-0
CMF Cl O4



IT **12150-46-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction by, of norbornadiene **rhodium** complex)
RN 12150-46-8 HCAPLUS
CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



L104 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1985:471462 HCAPLUS
DN 103:71462
ED Entered STN: 07 Sep 1985
TI 1,1'-Bis(alkylarylphosphino)ferrocenes: synthesis, metal complex formation, and crystal structure of three metal complexes of Fe(η5-C5H4PPh2)2
AU Butler, Ian R.; Cullen, William R.; Kim, Tae Jeong; Rettig, Steven J.; Trotter, James
CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
SO Organometallics (**1985**), 4(6), 972-80
CODEN: ORGND7; ISSN: 0276-7333
DT Journal
LA English
CC 29-12 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
OS CASREACT 103:71462
GI For diagram(s), see printed CA Issue.
AB The ferrocenylbisphosphines I (R = PR2R3; R1 = PR4R5) (R2-R5 = Ph or Me3C) were prepared by treating either dilithio I (R = R1 = Li) or I (R = Li, R1 = PR4R5 (II) with ClPR2R3. II was obtained by cleaving ferrocenophane I (RR1 = PR4) with R5Li. Best results were obtained when R4 and/or R5 = Ph. A range of PdLCl2, NiLX2, and [Rh(L)(NBD)]ClO4 [L = I; R1, R2 = PPh2, P(CMe3)2, PPhCMe3; NBD = norbornadiene; X = Cl, Br] complexes were prepared The crystal structures of PdLCl2, NiLBr2, and MoL(CO)4 (L = I; R = R1 = PPh2) showed the metal atoms had cis-square planar, tetrahedral, and cis-octahedral coordination, resp. The I (R = R1 = PPh2) ligands have slightly nonparallel cyclopentadienyl rings, with approx. staggered arrangements in the Pd and Mo compds. but an approx. eclipsed conformation in the Ni complex, with significant displacements of the P atoms from the ring planes. ML(CO)4 (M = Mo, Cr; L = I; R = R1 = PPh2) are fluxional in solution to -80°.
ST crystal structure ferrocenyl bisphosphine metal complex; mol structure ferrocenyl bisphosphine metal complex; phosphinoferrocene metal complex crystal structure; molybdenum bisphosphinoferrocene complex crystal structure; palladium bisphosphinoferrocene complex crystal structure; nickel bisphosphinoferrocene complex crystal structure; fluxionality chromium molybdenum bisphosphinoferrocene complex
IT Crystal structure
Molecular structure
(of bisphosphinoferrocene metal complexes)
IT Fluxional rearrangement
(of chromium or molybdenum bisphosphinoferrocene complexes)
IT 95408-44-9
RL: PRP (Properties)
(crystal structure of)
IT 67292-28-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluxionality and mol. structure of)
IT 67292-31-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluxionality of)
IT 83547-83-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reaction of, with chlorophosphines)
IT 72954-06-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reactions of, with chlorophosphine)
IT 67292-33-5P 95464-05-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
IT 72287-26-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

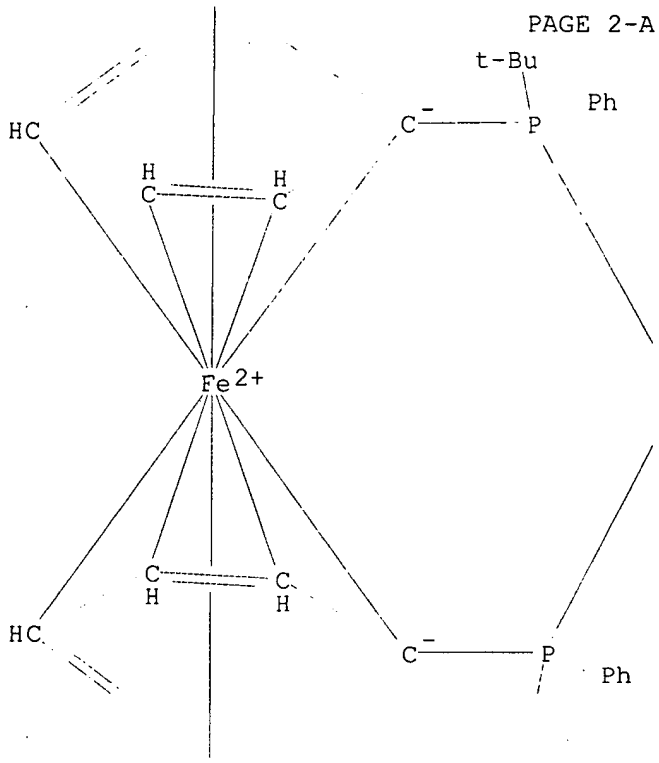
IT 95408-39-2P 95408-40-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with metal complex)
IT 95408-38-1P 95464-04-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of, with metal complexes)
IT 12098-17-8P **92269-95-9P 92284-07-6P** 95408-41-6P
95408-42-7P 95408-45-0P 95408-46-1P 95408-47-2P 95408-48-3P
95408-49-4P 95408-51-8P 95408-52-9P 95420-22-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 1079-66-9 13716-10-4 29949-69-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, for lithiated phosphinoferrocene)
IT 10025-98-6 12107-56-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bisphosphinoferrocene complexes)
IT 95408-37-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorophosphine)
IT 12150-46-8 84680-95-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with palladium or nickel complex)
IT 14220-64-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, with bisphosphinoferrocene complexes)
IT **92269-95-9P 92284-07-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 92269-95-9 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

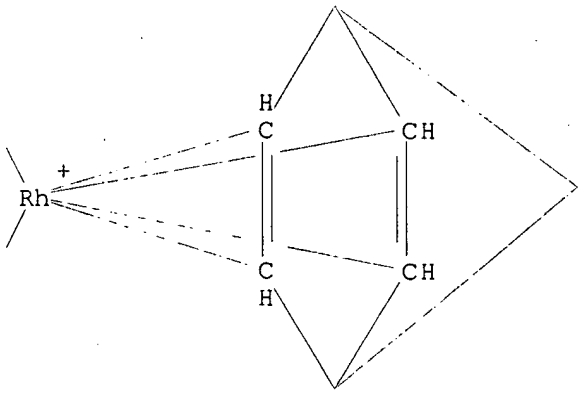
CRN 92269-94-8
CMF C37 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B

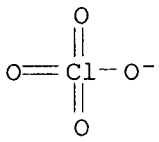


PAGE 3-A

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4



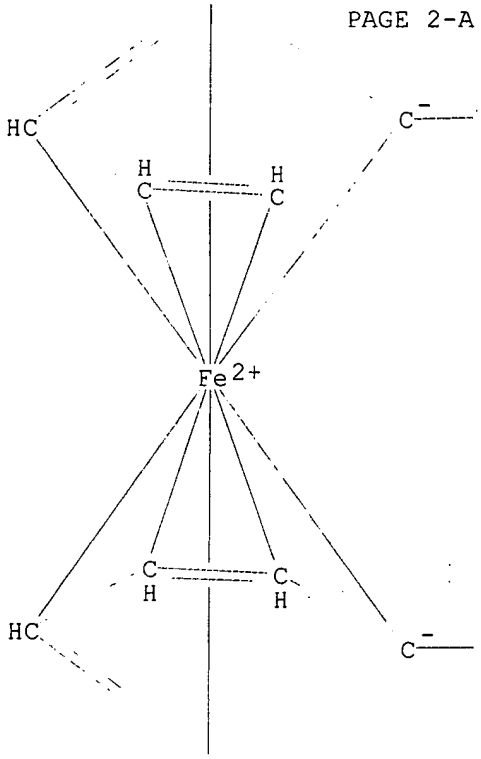
RN 92284-07-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

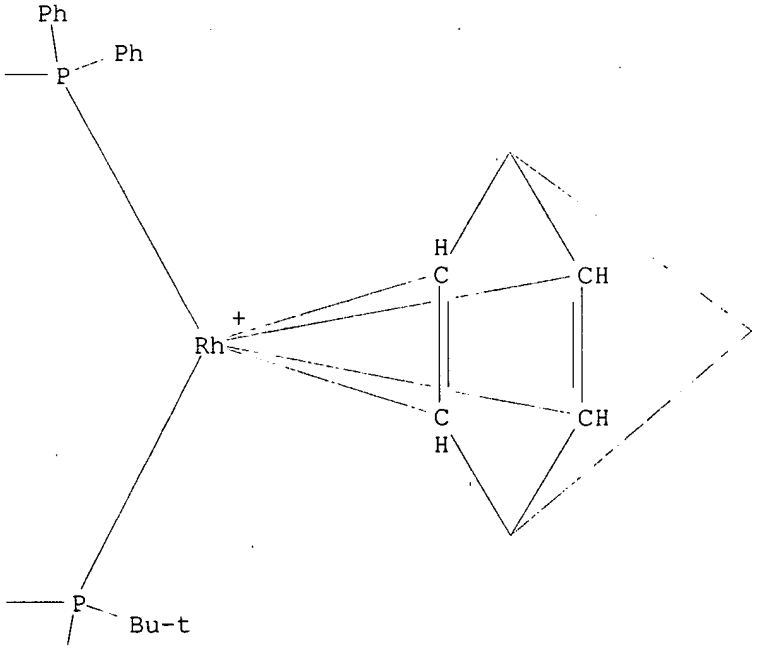
CRN 92284-06-5
CMF C37 H44 Fe P2 Rh
CCI CCS

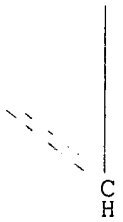
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B





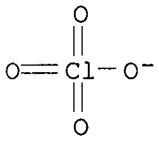
PAGE 3-A

PAGE 3-B

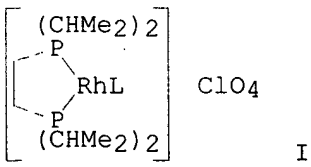
t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4



L104 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:185249 HCAPLUS
DN 102:185249
ED Entered STN: 02 Jun 1985
TI **Hydrogenation** of cationic bis(tertiary alkylphosphine) **rhodium**(I) complexes. An NMR study
AU Butler, Ian R.; Cullen, William R.; Mann, Brian E.; Nurse, Charles R.
CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
SO Journal of Organometallic Chemistry (**1985**), 280(2), C47-C50
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
GI



I

AB **Rhodium** hydrides have been observed in solution in the reaction of cationic **rhodium**(I) complexes of bis(tertiary phosphines), e.g., (I, L = norbornadiene) with H.
ST **hydrogenation phosphinerhodium** complex;

rhodium phosphine **hydrogenation**; hydride **rhodium** phosphine; NMR **hydrogenation phosphinerhodium** complex

IT Nuclear magnetic resonance
(of **hydrogenation** of **rhodium** phosphine complexes)

IT **Hydrogenation**
(of **rhodium** phosphine complexes)

IT **84680-96-6 92269-95-9** 96144-39-7 **96144-63-7 96144-65-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)

IT 96144-41-1P **96144-67-1P 96144-69-3P 96144-71-7P 96144-73-9P 96144-75-1P 96144-77-3DP**, perchlorate derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **84680-96-6 92269-95-9 96144-63-7 96144-65-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)

RN 84680-96-6 HCAPLUS

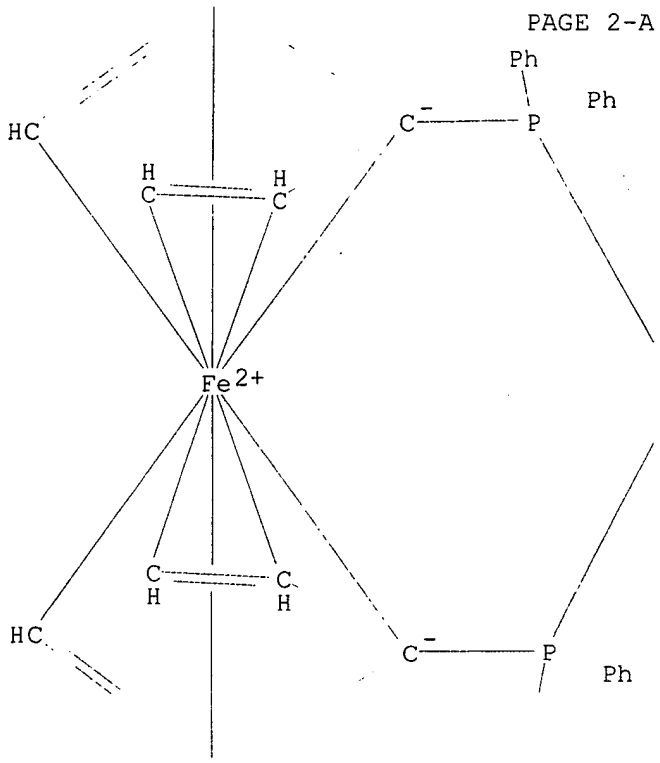
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

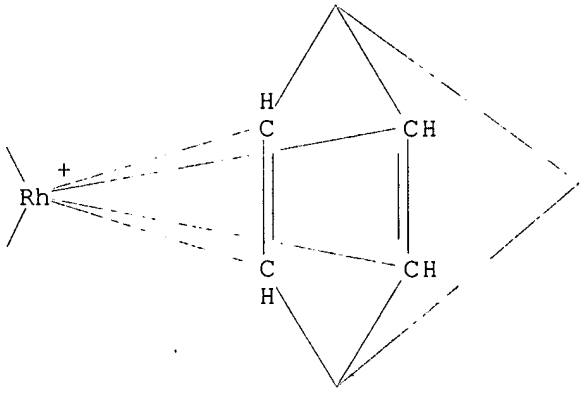
CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

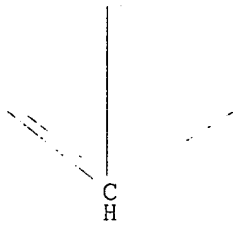
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B

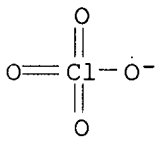




PAGE 3-A
Ph

CM 2

CRN 14797-73-0
CMF Cl O4



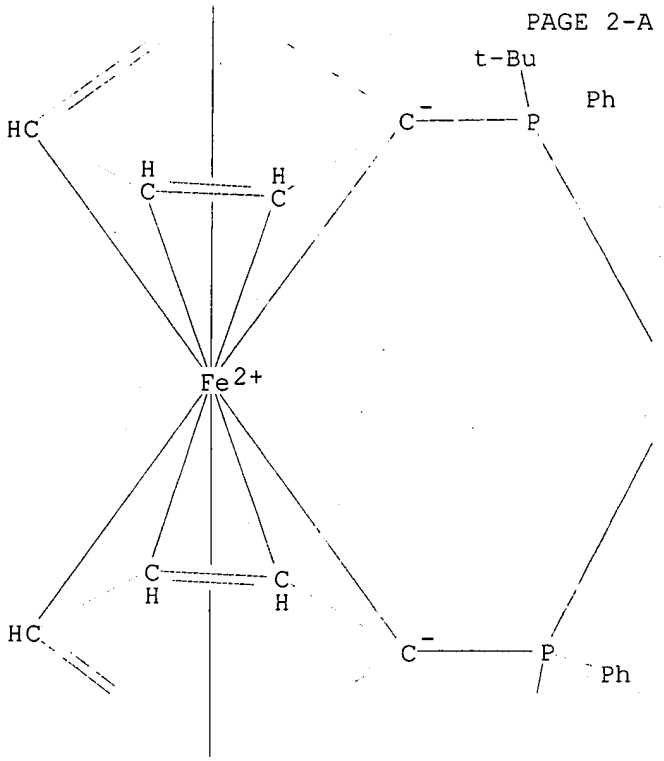
RN 92269-95-9 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 92269-94-8
CMF C37 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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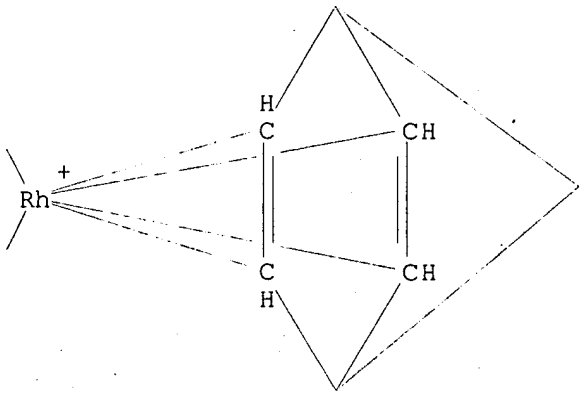
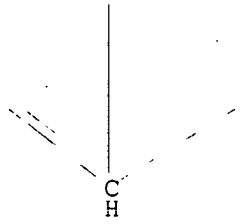


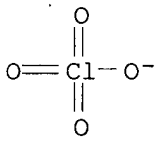


PAGE 3-A

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4



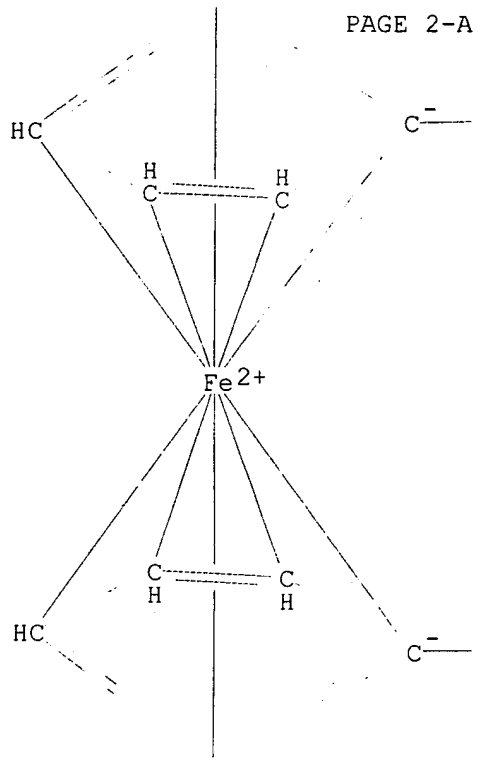
RN 96144-63-7 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-62-6
CMF C29 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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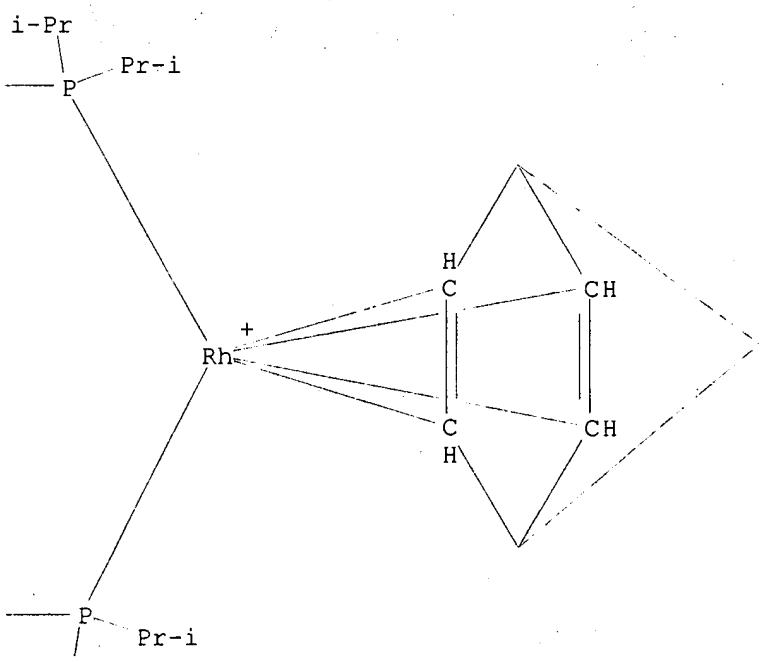


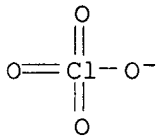
PAGE 3-A

PAGE 3-B

i-Pr

CM 2

CRN 14797-73-0
CMF Cl O4



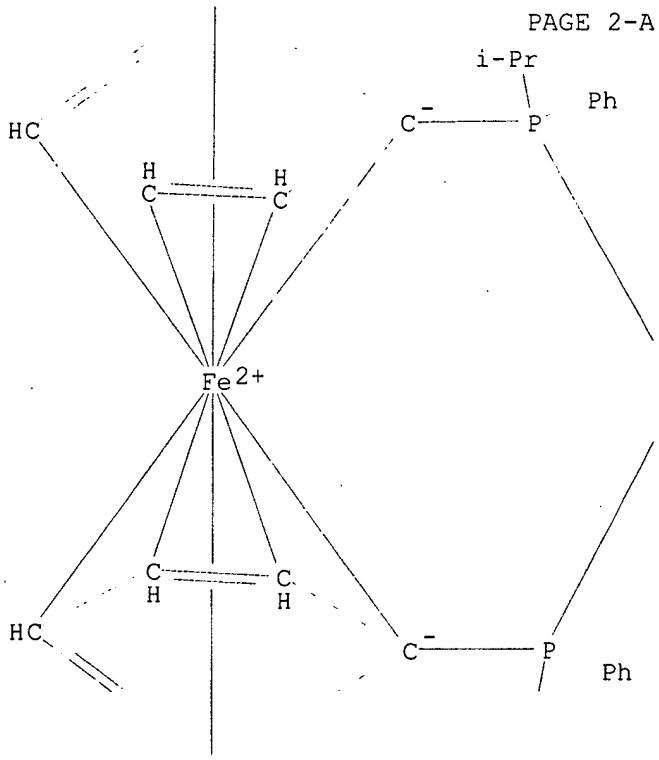
RN 96144-65-9 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1-methylethyl)phenylphosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-64-8
CMF C35 H40 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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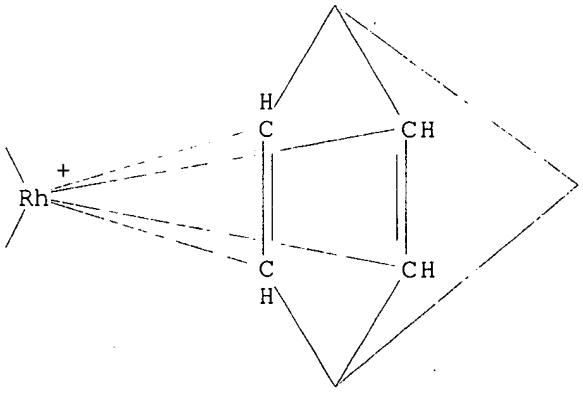
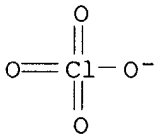


PAGE 3-A

i-Pr

CM 2

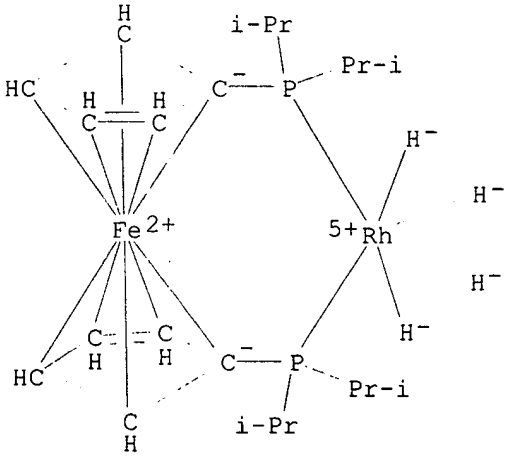
CRN 14797-73-0
CMF Cl O4



IT **96144-67-1P 96144-69-3P 96144-71-7P**
96144-73-9P 96144-75-1P 96144-77-3DP,
perchlorate derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 96144-67-1 HCAPLUS
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']tetrahydro-, perchlorate (9CI) (CA INDEX NAME)

CM 1

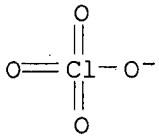
CRN 96144-66-0
CMF C22 H40 Fe P2 Rh
CCI CCS



CM 2

CRN 14797-73-0

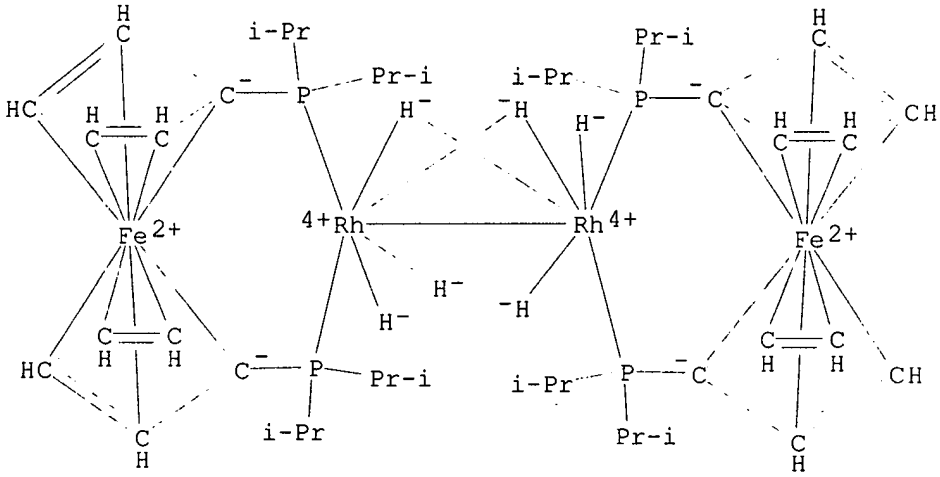
CMF Cl O4



RN 96144-69-3 HCAPLUS
CN Rhodium(2+), bis[1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']di-μ-hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

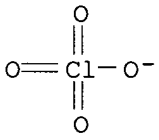
CM 1

CRN 96144-68-2
CMF C44 H78 Fe2 P4 Rh2
CCI CCS



CM 2

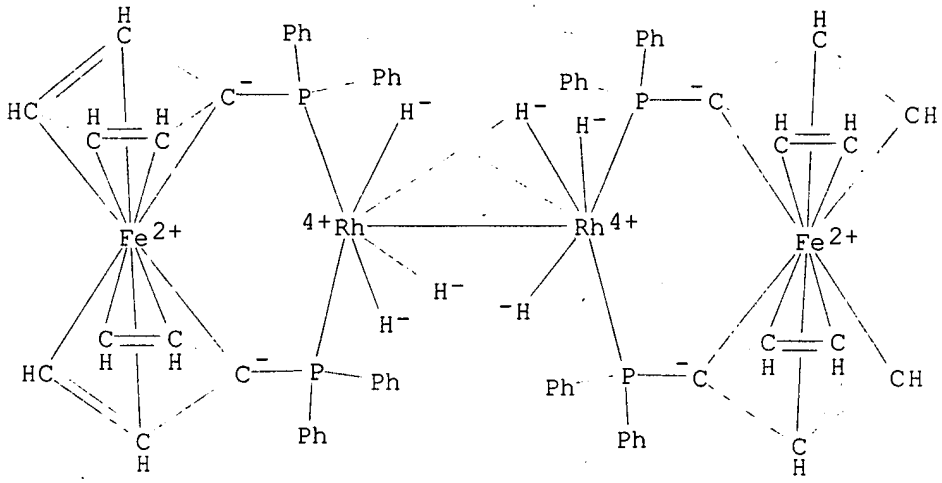
CRN 14797-73-0
CMF Cl O4



RN 96144-71-7 HCAPLUS
CN Rhodium(2+), bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di-μ-hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

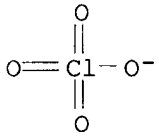
CM 1

CRN 96144-70-6
CMF C68 H62 Fe2 P4 Rh2
CCI CCS



CM 2

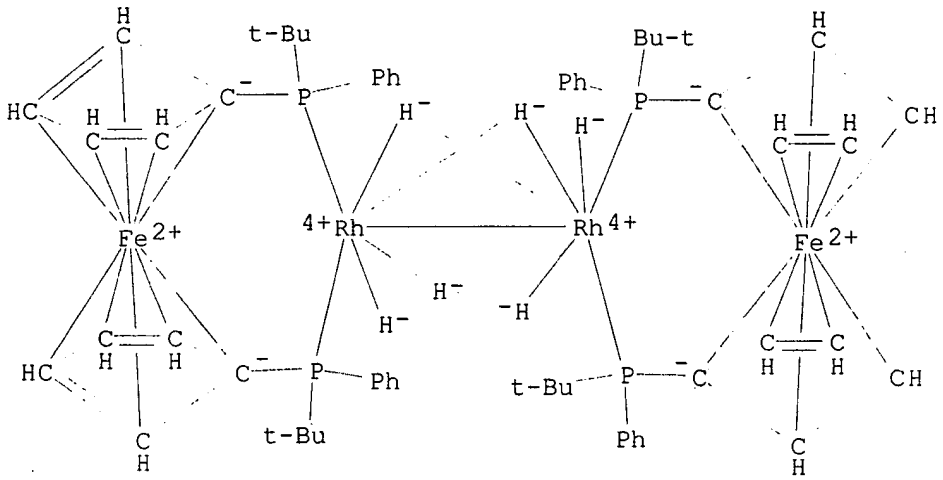
CRN 14797-73-0
CMF Cl O4



RN 96144-73-9 HCAPLUS
CN Rhodium(2+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']di-μ-hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

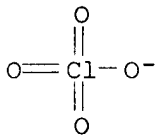
CM 1

CRN 96144-72-8
CMF C60 H78 Fe2 P4 Rh2
CCI CCS



CM 2

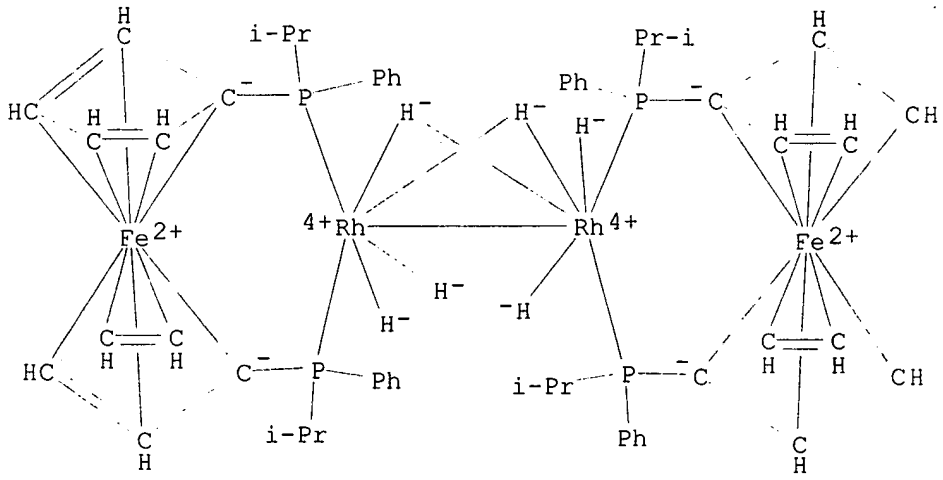
CRN 14797-73-0
CMF Cl O4



RN 96144-75-1 HCAPLUS
CN Rhodium(2+), bis[1,1'-bis[(1-methylethyl)phenylphosphino]ferrocene-P,P']di-μ-hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

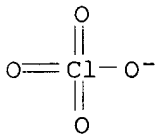
CM 1

CRN 96144-74-0
CMF C56 H70 Fe2 P4 Rh2
CCI CCS



CM 2

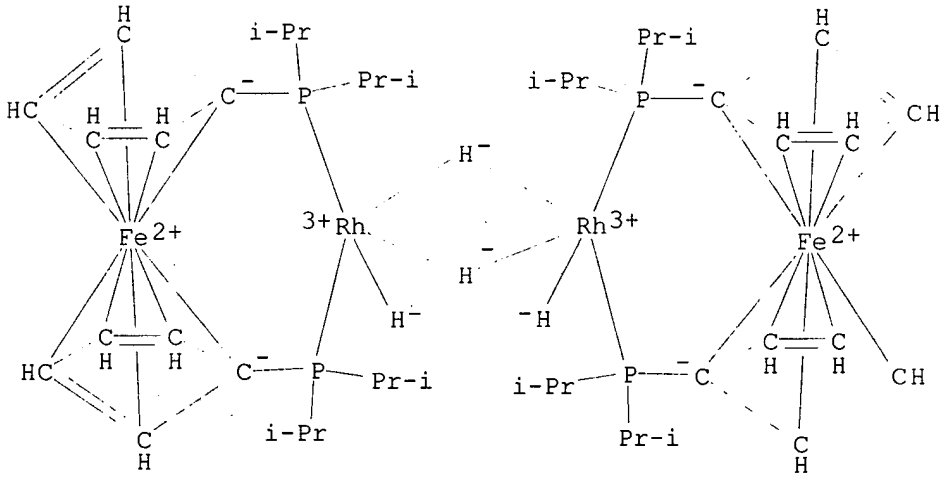
CRN 14797-73-0
CMF Cl O4



RN 96144-77-3 HCAPLUS
CN Rhodium(2+), bis[1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']di-μ-hydrodihydrodi-, diperchlorate (9CI) (CA INDEX NAME)

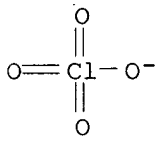
CM 1

CRN 96144-76-2
CMF C44 H76 Fe2 P4 Rh2
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4



L104 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:166925 HCAPLUS
DN 102:166925

ED Entered STN: 18 May 1985
TI **Rhodium**(I) complexes of ferrocenylphosphines as efficient asymmetric catalysts. The structure of Fe(η5-C5H3(P(CMe3)2-1,3)(η5-C5H3(CHMeNMe2)P(CMe3)2-1,2)
AU Appleton, Trevor D.; Cullen, William R.; Evans, Stephen V.; Kim, Tae Jeong; Trotter, James
CS Dep. Chem., Univ. Br. Columbia, Vancouver, BC, V6T 1Y6, Can.
SO Journal of Organometallic Chemistry (**1985**), 279(1-2), 5-21
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23, 25, 67, 75
OS CASREACT 102:166925
GI For diagram(s), see printed CA Issue.
AB The chiral aminomethylferrocenes (R)- or (S)-I (R-R2 = H) were lithiated and treated with ClP(CMe3)2 under varying reaction conditions to give (R,S)-I [R = P(CMe3)2; R1 = H (II), P(CMe3)2 (III); R2= H] and (S,R)-I (same R's) resp. Similarly, (R, R)- or (S, S)-I [R = R2 = P(CMe3)2, R1 = H] (IV) were prepared from (R)- or (S)-I (R-R2 = H) resp. [**Rh**(NBD)L]ClO4 [V; NBD = norbornadiene, L = (S,R)-II, (S,R-III, (S,S)-IV] catalyzed asym **hydrogenation** of H2C:CR3CO2H (R3 = Me, CH2CO2H) and PhCH:CR4CO2H (R4 = NHAc, Me); V [L = (S,S)-IV] gave products with up to 95% enantiomeric excesses. The x-ray crystal structure of (S,S)-IV showed the cyclopentadienyl rings are close to planar, deviate slightly from coplanarity, and are rotated by about 7° from an eclipsed conformation. The substituent P and C atoms are significantly displaced from the ring planes.
ST crystal structure ferrocenyltriphosphine chiral; mol structure ferrocenyltriphosphine chiral; ferrocenylphosphine structure **rhodium** complex catalyst; **rhodium** ferrocenylphosphine complex **hydrogenation** asym
IT Crystal structure
Molecular structure
(of ferrocenyltriphosphine complex, chiral)
IT Asymmetric synthesis and induction
(of organic acids, by **hydrogenation** of olefinic acids, **rhodium**-ferrocenylphosphine catalyst for)
IT **Hydrogenation**
(asym., of olefinic acids)
IT **Hydrogenation catalysts**
(asym., **rhodium**-ferrocenyltriphenylphosphine complex, for olefinic acids)
IT 97-65-4, reactions 1895-97-2 5429-56-1 55065-02-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. **hydrogenation** of, **rhodium**-ferrocenylphosphine complex for)
IT 95840-92-9
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for asym. **hydrogenation** of olefinic acids)
IT 83356-93-8 95839-80-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of, with **rhodium** complex)
IT 31886-57-4 31886-58-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and phosphination of)
IT **95762-74-6P 95839-79-5P 95840-91-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with **rhodium**)
IT **95839-76-2P 95839-78-4P** 95840-90-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation of)
IT 97-69-8P 2018-61-3P 2174-58-5P 3641-51-8P 10172-89-1P

14367-54-5P 14367-67-0P 19436-52-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by asym. **hydrogenation** of olefinic acid, **rhodium**-ferrocenyltriphosphine complex for)

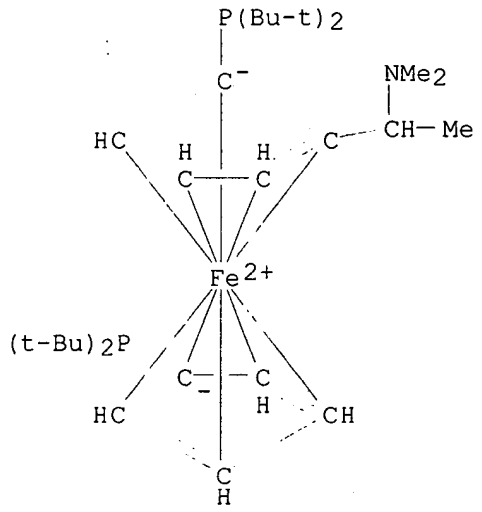
IT **95762-71-3P 95762-73-5P** 95840-45-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, conformation, and catalyst activity of, for asym. **hydrogenation**)

IT **95762-75-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, and complexation of, with **rhodium**)

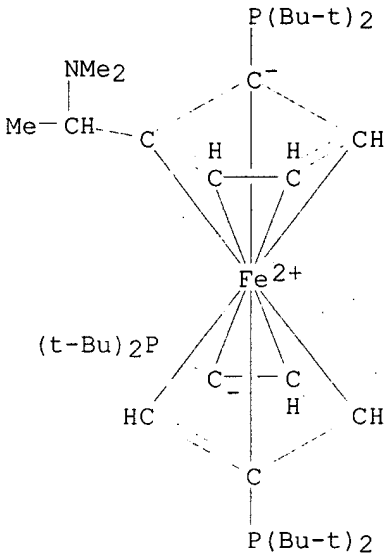
IT 13716-10-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chiral aminoferrocene)

IT **95762-74-6P 95839-79-5P 95840-91-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with **rhodium**)

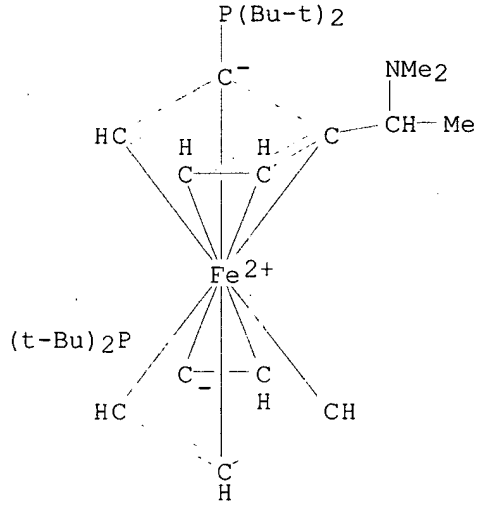
RN 95762-74-6 HCAPLUS
CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)



RN 95839-79-5 HCAPLUS
CN Ferrocene, 1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)



RN 95840-91-8 HCAPLUS
CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

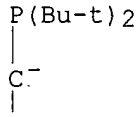


IT **95839-76-2P 95839-78-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation of)
RN 95839-76-2 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-N2,P1]-, [R-(R*,R*)]-, perchlorate (9CI) (CA INDEX NAME)

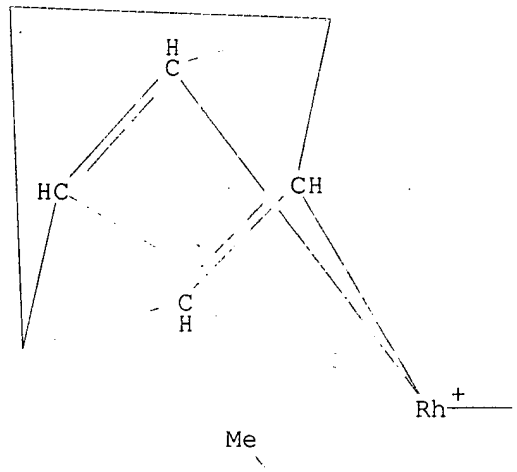
CM 1

CRN 95839-75-1
CMF C37 H61 Fe N P2 Rh
CCI CCS

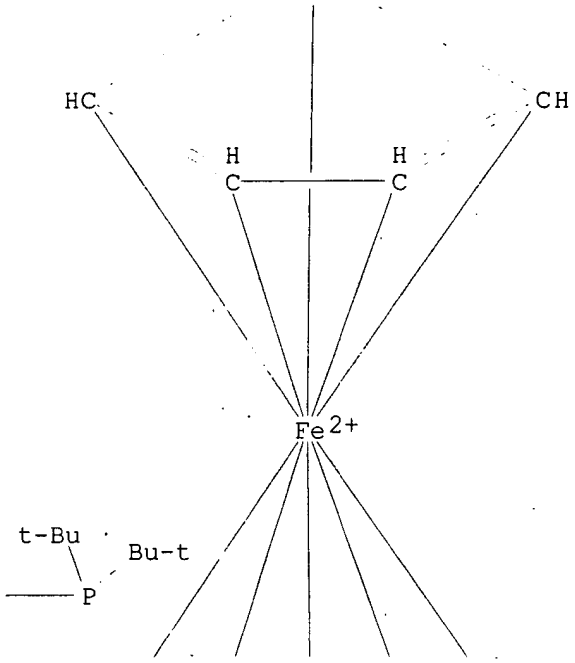
PAGE 1-B



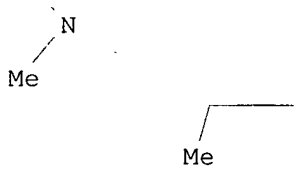
PAGE 2-A



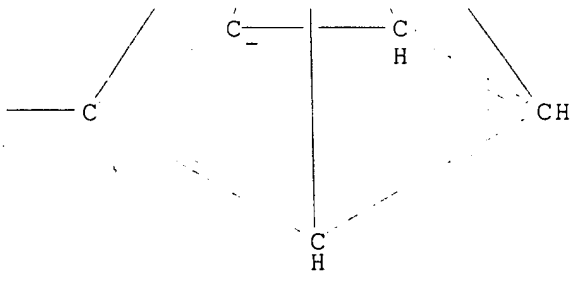
PAGE 2-B



PAGE 3-A

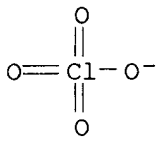


PAGE 3-B



CM 2

CRN 14797-73-0
CMF Cl O4

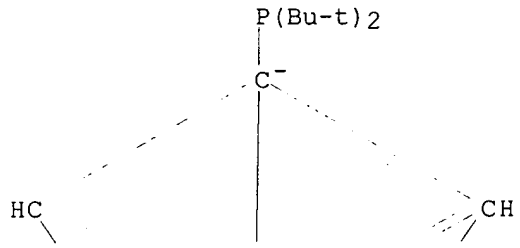


RN 95839-78-4 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-N2,P1]-, [S-(R*,S*)]-, perchlorate (9CI) (CA INDEX NAME)

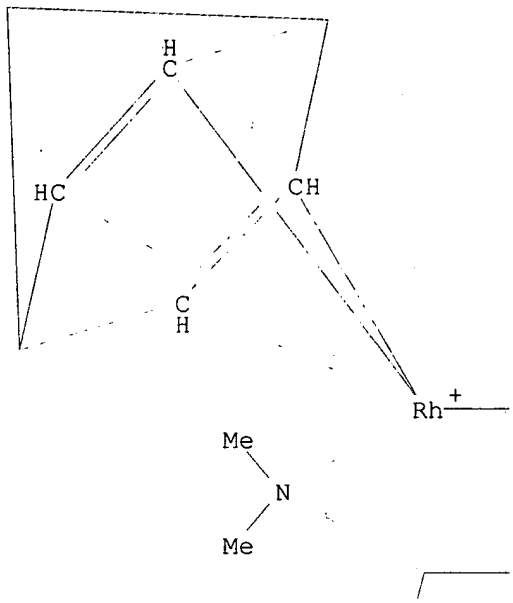
CM 1

CRN 95839-77-3
CMF C45 H78 Fe N P3 Rh
CCI CCS

PAGE 1-B



PAGE 2-A



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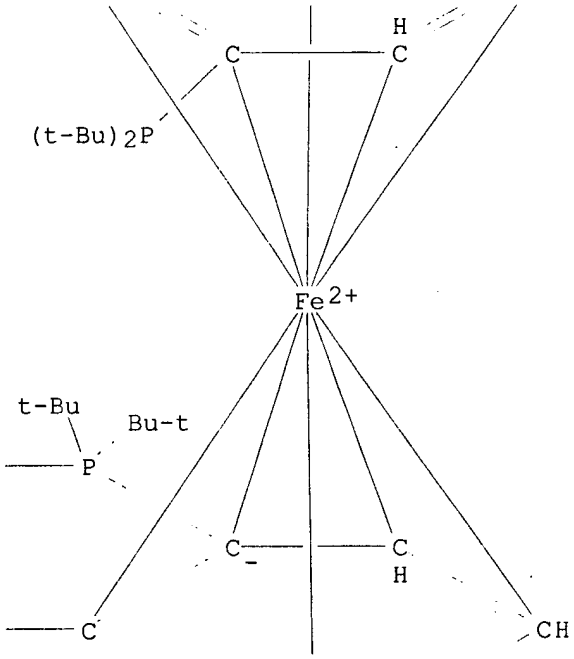


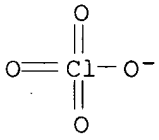
PAGE 3-A

Me

PAGE 3-B

CM 2

CRN 14797-73-0
CMF Cl O4

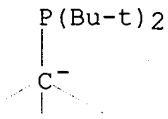


IT **95762-71-3P 95762-73-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, conformation, and catalyst activity of, for asym. **hydrogenation**)
RN 95762-71-3 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-N2,P1]-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 95762-70-2
CMF C37 H61 Fe N P2 Rh
CCI CCS

PAGE 1-B



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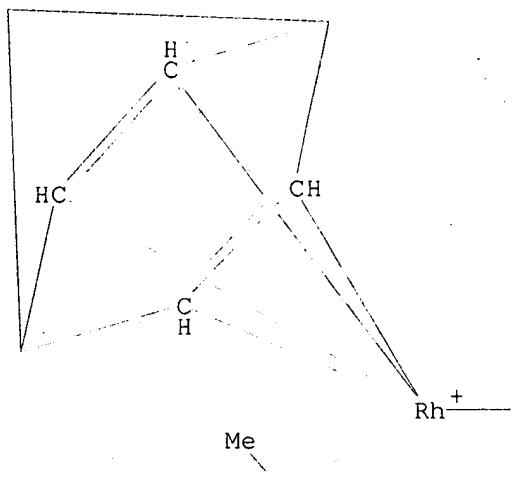

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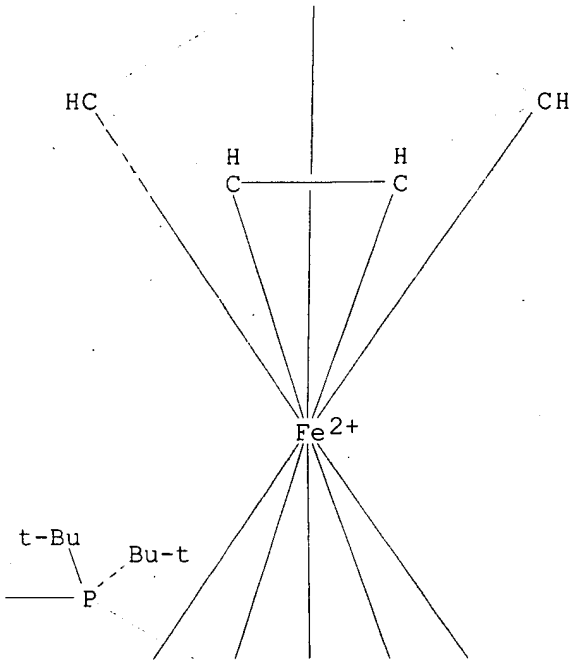

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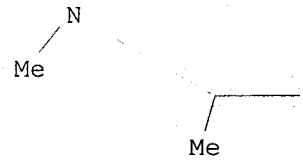

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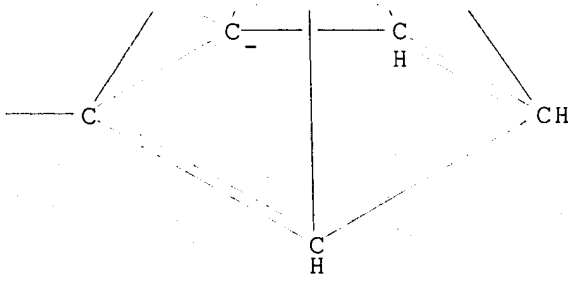
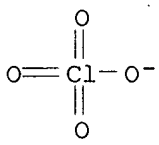


CM 2

CRN 14797-73-0
CMF Cl O4

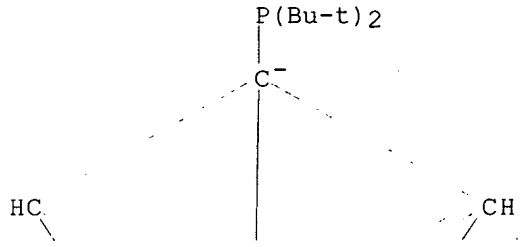


RN 95762-73-5 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1',3-tris[bis(1,1-dimethylethyl)phosphino]-2'-[1-(dimethylamino)ethyl]ferrocene-N2',P1']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 95762-72-4
CMF C45 H78 Fe N P3 Rh
CCI CCS

PAGE 1-B



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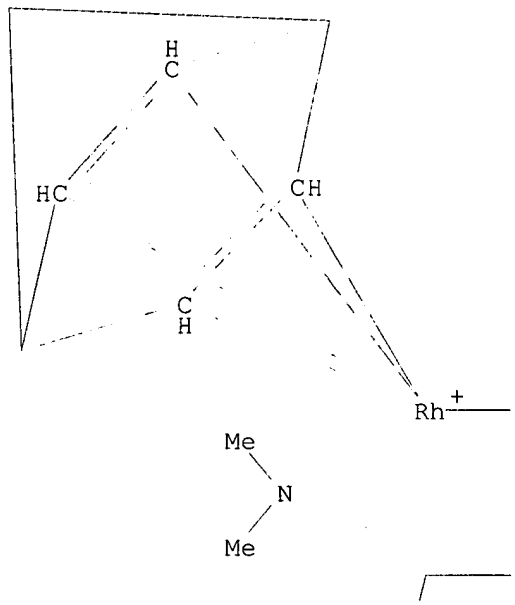

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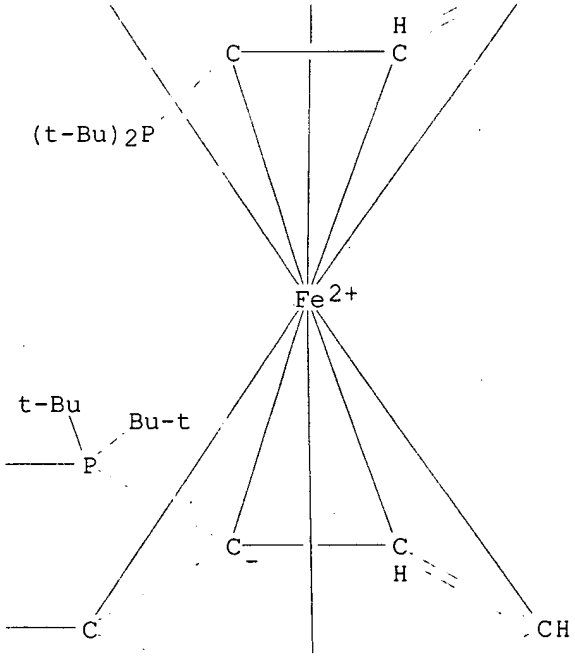


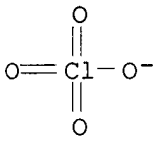
PAGE 3-A

Me

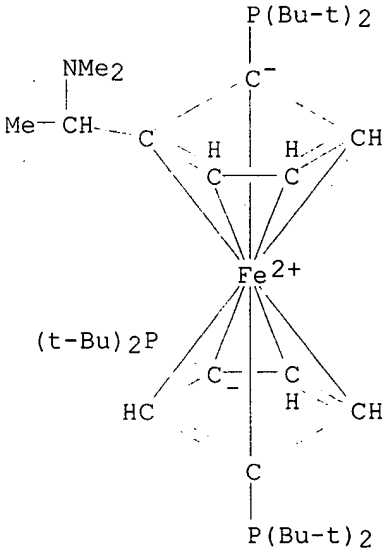
PAGE 3-B

CM 2

CRN 14797-73-0
CMF Cl O4



IT **95762-75-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, and complexation of, with **rhodium**
)
RN 95762-75-7 HCAPLUS
CN Ferrocene, 1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)



L104 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:158448 HCAPLUS
DN 102:158448
ED Entered STN: 04 May 1985
TI Crystallographic analysis of two rhodium(III) hydride complexes, bis{1,1'-bis[tert-butyl(phenyl)phosphino]ferrocene-P,P'}-tri-μ-hydrido-

dihydridodirhodium(III) chlorate methanol solvate, [Rh2H5{Fe[P(C4H9)(C5H4)(C6H5)]2}2]ClO4.CH3OH (I), and bis[1,1'-bis(di-tert-butylphosphino)ferrocene-P,P']-tri-μ-hydrido-dihydridodirhodium(III) chlorate, [Rh2H5{Fe[P(C4H9)2(C5H4)]2}2]ClO4 (II)

AU Einstein, F. W. B.; Jones, T.

CS Dep. Chem., Simon Fraser Univ., Burnaby, BC, V5A 1S6, Can.

SO Acta Crystallographica, Section C: Crystal Structure Communications (1985), C41(3), 365-9
CODEN: ACSCEE; ISSN: 0108-2701

DT Journal

LA English

CC 75-8 (Crystallography and Liquid Crystals)
Section cross-reference(s): 29, 78

AB Title compound (I) is monoclinic, space group P21/n, with a 18.708(4), b 14.857(2), c 21.853(4) Å, and β 92.95(2)°; Z = 4 for d = 1.501. The final R = 0.045 for 5732 reflections. Title compound (II) is monoclinic, space group P21/c, with a 15.276(3), b 14.751(2), c 25.950(3) Å, and β 90.85(1)°; Z = 4, for d = 1.430. The final R = 0.059 for 4180 reflections. The structure of I contains an unusual RhPH skeletal structure in which each Rh atom (in the 3+ oxidation state) has 3 Rh-H bridging bonds [average 1.77(8) Å], a single Rh-H terminal bond [average 1.56(12) Å] and 2 Rh-P bonds. It is tentatively proposed that II contains a similar arrangement. Atomic coordinates are given.

ST mol structure rhodium hydro bridged phosphinoferrocene; ferrocene butylphosphino rhodium hydro structure

IT Crystal structure
Molecular structure
(of rhodium hydro-bridged butylphenylphosphinoferrocene and dibutylphosphinoferrocene complexes)

IT **92468-68-3** 95783-24-7
RL: PRP (Properties)
(structure of)

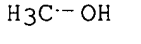
IT **92468-68-3**
RL: PRP (Properties)
(structure of)

RN 92468-68-3 HCAPLUS

CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, stereoisomer, perchlorate, compd. with methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1
CMF C H4 O

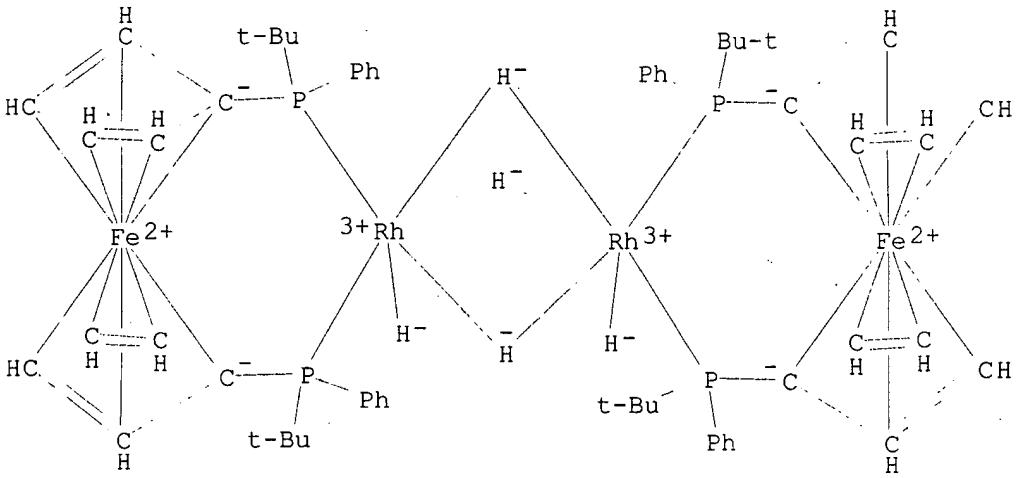


CM 2

CRN 92468-67-2
CMF C60 H77 Fe2 P4 Rh2 . Cl O4

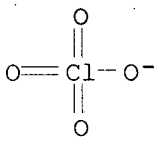
CM 3

CRN 92468-66-1
CMF C60 H77 Fe2 P4 Rh2
CCI CCS



CM 4

CRN 14797-73-0
CMF Cl O4



L104 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:79103 HCAPLUS
DN 102:79103
ED Entered STN: 09 Mar 1985
TI Structures of three **hydrogenation** catalysts [(P-P)**Rh**(NBD)]ClO4 and some comparative rate studies where (P-P) = (η5-R1R2PC5H4)(η5-R3R4PC5H4)Fe (R1 = R2 = R3 = R4 = Ph; R1 = R2 = Ph, R3 = R4 = CMe3; R1 = R3 = Ph, R2 = R4 = CMe3)
AU Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W. B.; Jones, Terry
CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
SO Organometallics (**1985**), 4(2), 346-51
CODEN: ORGND7; ISSN: 0276-7333
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22
AB Bulky Me3C groups enhance the **hydrogenation** rates of alkenes (except for bulky substrates) at 30°/1 atm H2 using the title compds. [(P-P)RhNBD]ClO4 [(P-P) = (η5-R1R2PC5H4)Fe(η5-R3R4PC5H4); R1 =R2 = R3 = R4 = Me3C (I), Ph (II); R1 = R2 = Me3C, R3 = R4 = Ph (III); R1 = R3 = Me3C, R2 = R4 = Ph (IV)] as catalyst precursors. The most promising combination of steric and electronic effects exists with (±)-IV. Crystallog. of II, III, and IV show that the bulky Me3C groups cause a lengthening of P-**Rh** distances, wider P-**Rh**-P angles, and a rotation of the norbornadiene group out of the P-**Rh**-P plane. Generally the effects range from a maximum in I (previously determined)

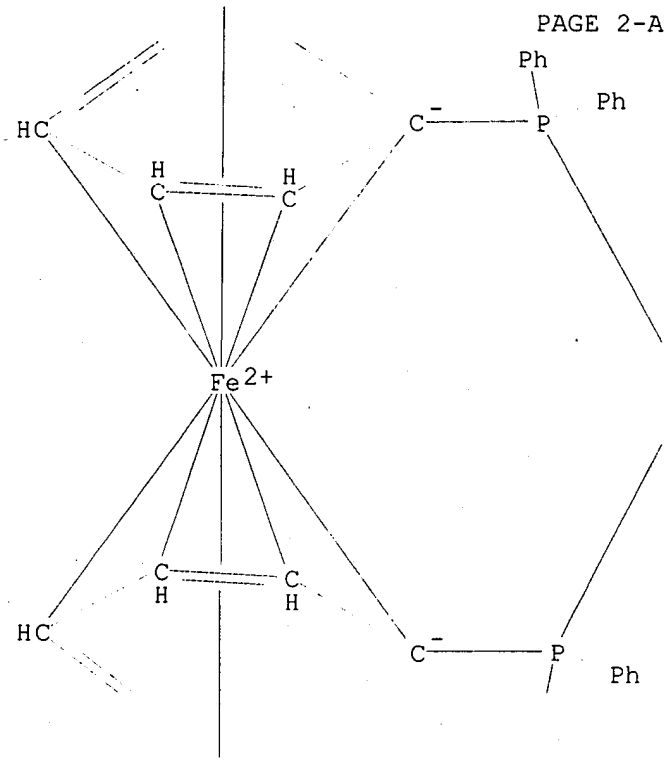
to a min. in II.
ST crystal structure **rhodium** phosphine complex; mol structure **rhodium** phosphine complex; steric effect **hydrogenation** catalyst; ferrocenebisphosphine **rhodium** complex butyl group
IT tert-Butyl group
(effect of, on **hydrogenation** of alkenes using ferrocenebis(phosphine)**rhodium** complex catalyst)
IT **Hydrogenation catalysts**
(ferrocenebis(phosphine) **rhodium** complexes, for alkenes, kinetics and mechanism with)
IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, **rhodium** phosphine catalyst for)
IT Bond angle
Bond length
(in ferrocenebis(phosphine) **rhodium** complexes)
IT Kinetics of **hydrogenation**
(of alkenes in presence of ferrocenebis(phosphine) **rhodium** complexes)
IT **Hydrogenation**
(of alkenes in presence of ferrocenebis(phosphine) **rhodium** complexes, mechanism of)
IT Crystal structure
Molecular structure
(of ferrocenebis(phosphine) **rhodium** complexes)
IT Substituent effect
(on catalytic activity of ferrocene bis(phosphine)**rhodium** complex in **hydrogenation** of alkenes)
IT Steric effect
(on **hydrogenation** of alkenes using ferrocenebis(phosphine) **rhodium** complexes)
IT **84680-96-6 92269-95-9 92284-07-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, crystallog. in relation to kinetics and mechanism with)
IT **84680-98-8**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, mol. structure in relation to kinetics and mechanism with)
IT 97-65-4, reactions 110-83-8, reactions 1199-77-5 5429-56-1 5469-45-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, using ferrocenebis(phosphine) **rhodium** complexes, kinetics and mechanism of)
IT **84680-96-6 92269-95-9 92284-07-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, crystallog. in relation to kinetics and mechanism with)
RN 84680-96-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

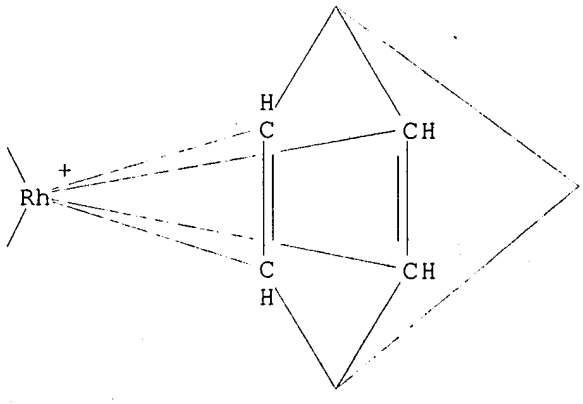
CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

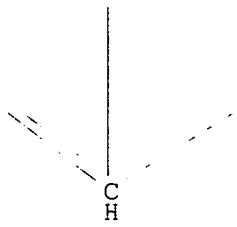
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



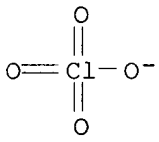


PAGE 3-A

Ph

CM 2

CRN 14797-73-0
CMF Cl O4



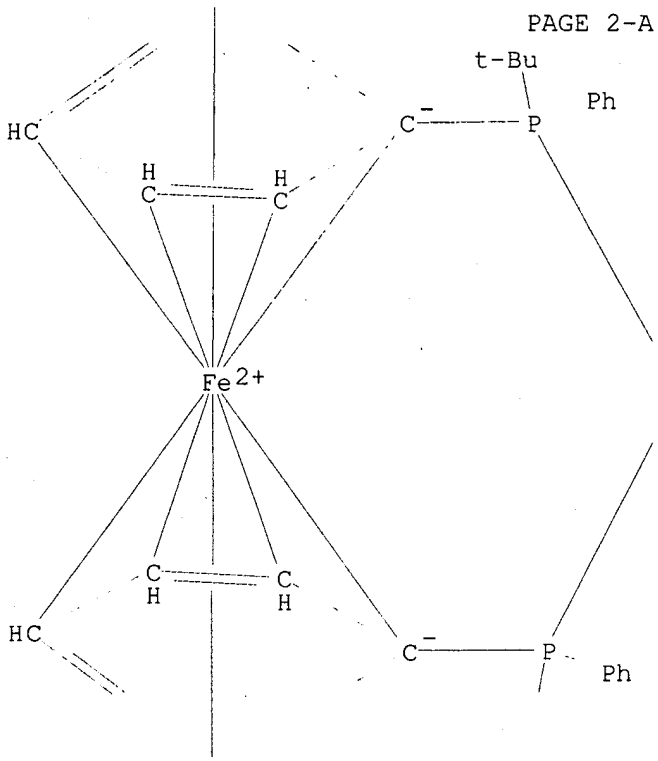
RN 92269-95-9 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

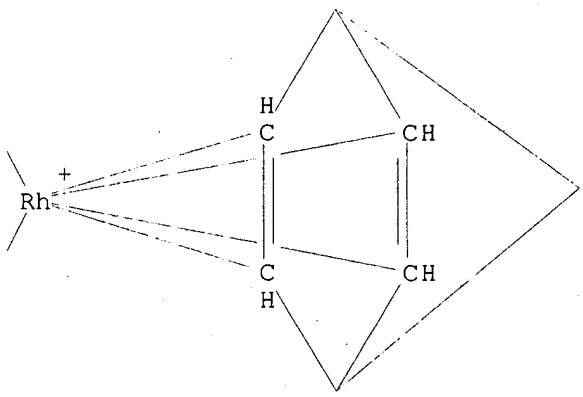
CRN 92269-94-8
CMF C37 H44 Fe P2 Rh
CCI CCS

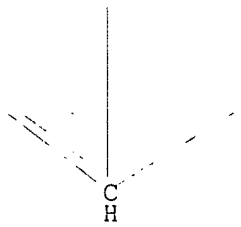
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



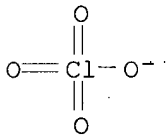


PAGE 3-A

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4



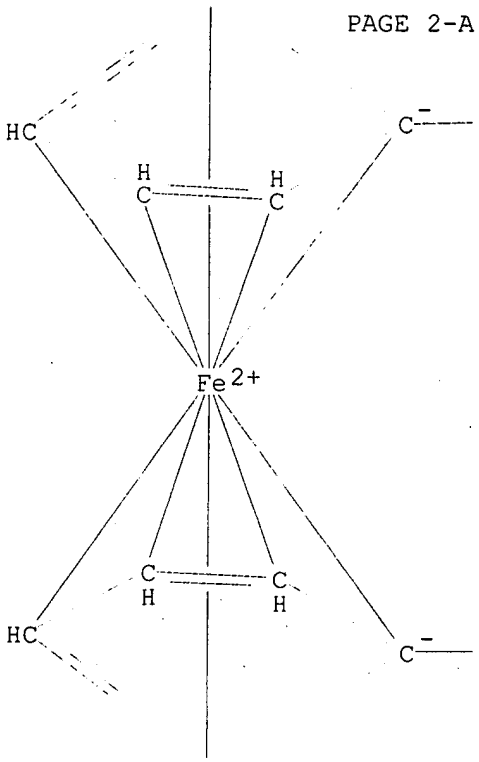
RN 92284-07-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 92284-06-5
CMF C37 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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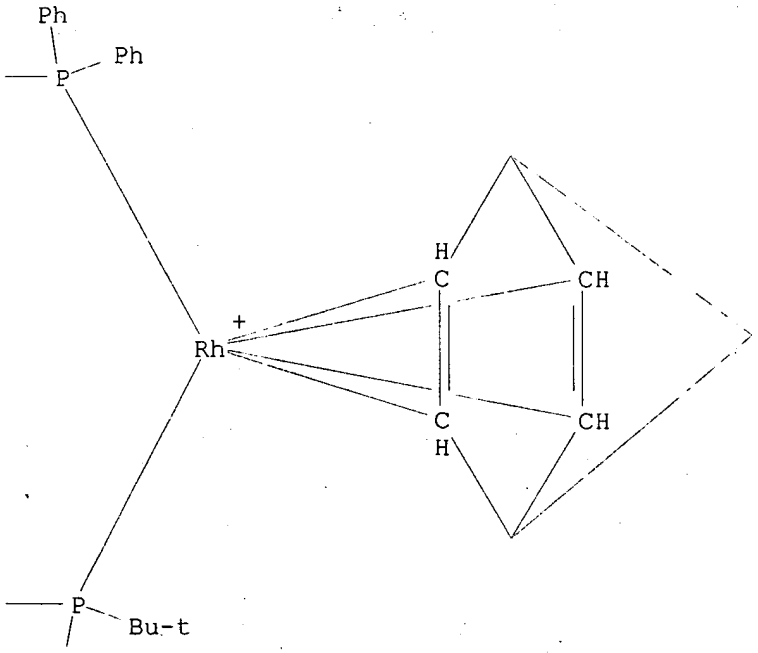
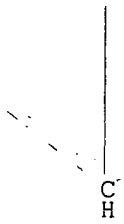




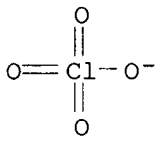
PAGE 3-A

PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4



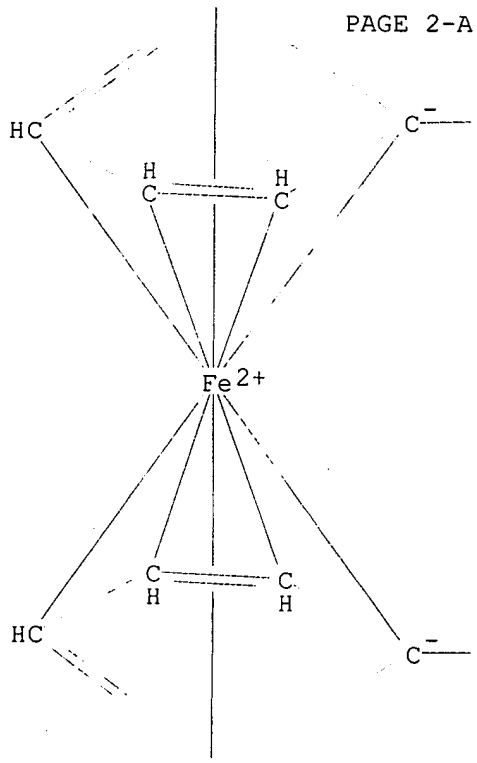
IT **84680-98-8**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, mol. structure in relation to kinetics and mechanism with)
RN 84680-98-8 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 84680-97-7
CMF C33 H52 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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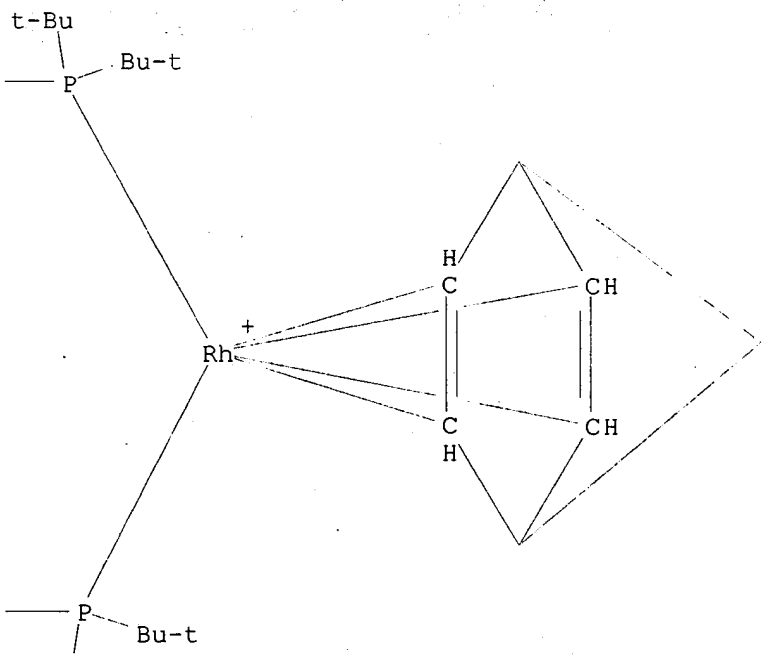
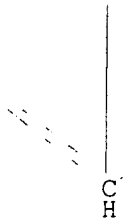




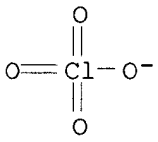
PAGE 3-A

PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4



L104 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:571461 HCAPLUS
DN 101:171461
ED Entered STN: 10 Nov 1984
TI Metal hydrides from cationic **rhodium**(I) catalyst precursors. X-ray structure of [(L-L)HRh(μ-H)3RhH(L-L)]ClO4 [L-L = rac-Fe(η5-C5H4PPhCMe3)2]
AU Butler, Ian R.; Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W. B.; Jones, Terry
CS Chem. Dep., Univ. British Columbia, Vancouver, V6T 1Y6, Can.
SO Journal of the Chemical Society, Chemical Communications (**1984**), (11), 719-21
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 67, 75
AB Treatment of [LRhL1]ClO4 [L = rac-Fe(η5-C5H4PPhCMe3)2, Fe[η5-C5H4P(CMe3)2]2 (C5H5 = cyclopentadienyl), L1 = norbornadiene] with H in MeOH at 30° and 1 atm gave [LHRh(μ-H)3RhLH]ClO4 (L as before) (II and III, resp.). The structures of II and III were determined by x-ray anal.
ST **rhodium** ferrocenylphosphine hydride crystal structure; catalyst **rhodium** ferrocenylphosphine **hydrogenation**
IT Crystal structure
Molecular structure
(of hydride-bridged **rhodium** ferrocenylphosphines)
IT **84680-98-8 92269-95-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)

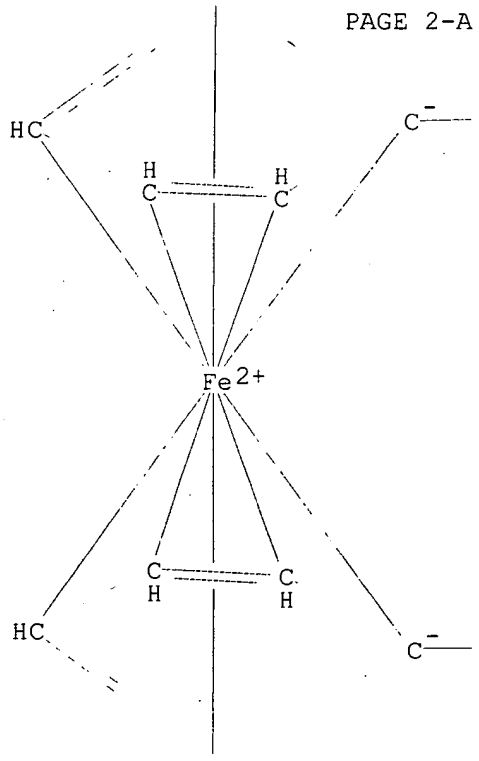
IT **92468-68-3P 92468-70-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure of)
IT **92468-67-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)
IT **84680-98-8 92269-95-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)
RN 84680-98-8 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 84680-97-7
CMF C33 H52 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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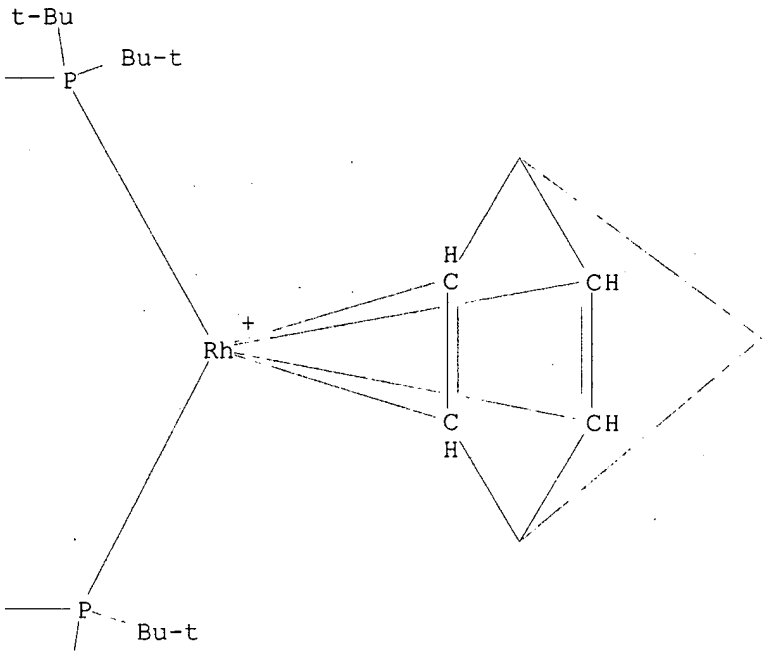


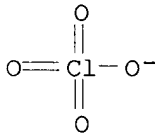
PAGE 3-A

PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4



RN 92269-95-9 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-

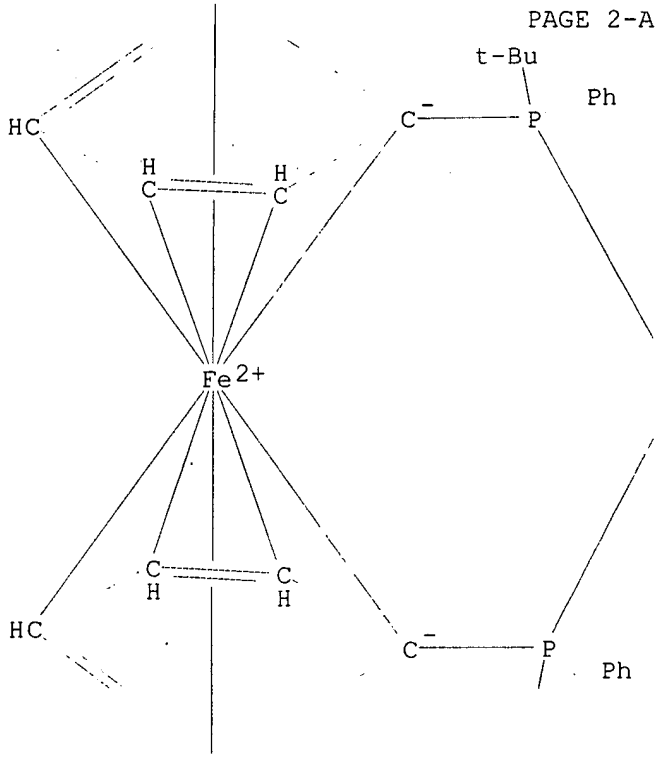
dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 92269-94-8
CMF C37 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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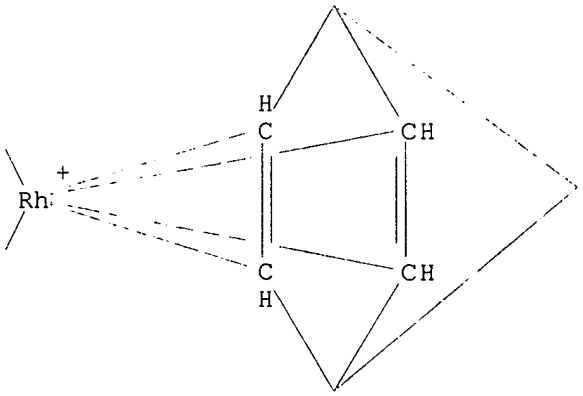

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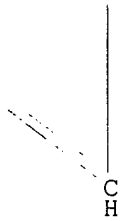
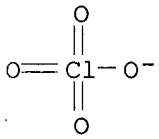


CM 2

CRN 14797-73-0
CMF Cl O4



IT **92468-68-3P 92468-70-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure of)
RN 92468-68-3 HCAPLUS
CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, stereoisomer, perchlorate, compd. with methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1
CMF C H4 O

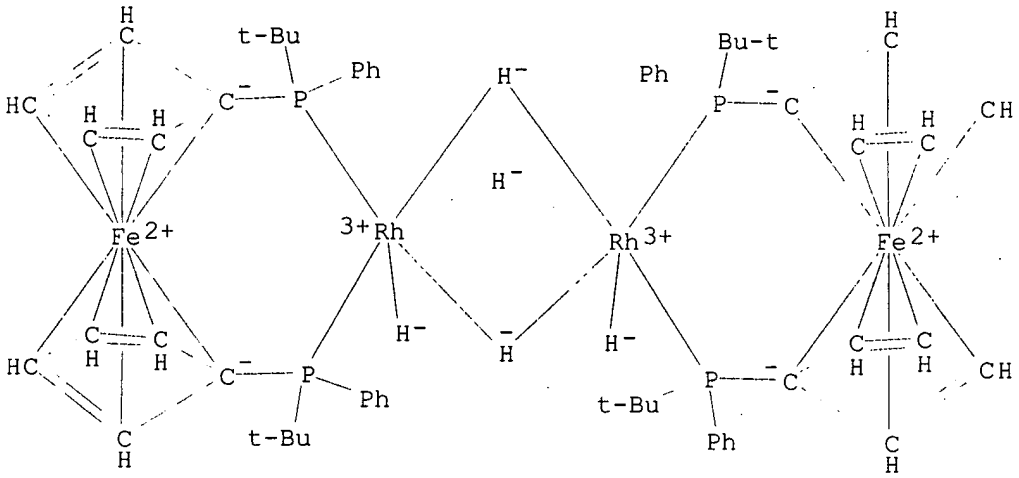
H_3C-OH

CM 2

CRN 92468-67-2
CMF C60 H77 Fe2 P4 Rh2 . Cl O4

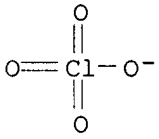
CM 3

CRN 92468-66-1
CMF C60 H77 Fe2 P4 Rh2
CCI CCS



CM 4

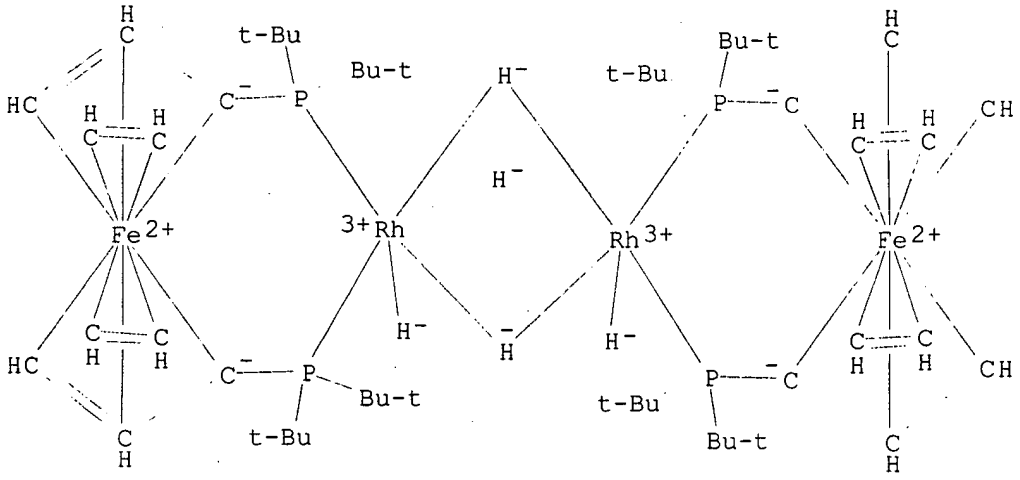
CRN 14797-73-0
CMF Cl O4



RN 92468-70-7 HCAPLUS
CN Rhodium(1+), bis[1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

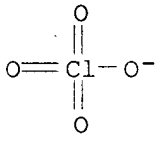
CM 1

CRN 92468-69-4
CMF C52 H93 Fe2 P4 Rh2
CCI CCS



CM 2

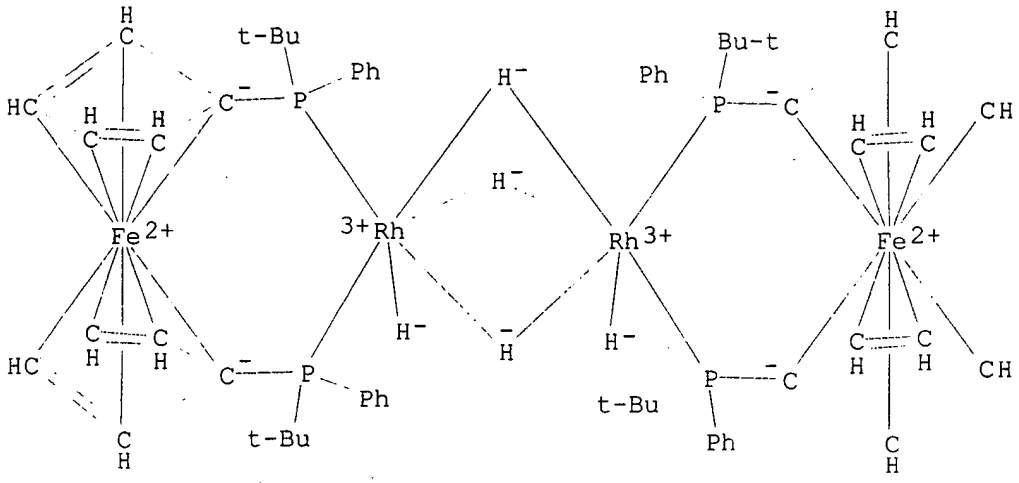
CRN 14797-73-0
CMF Cl O4



IT **92468-67-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)
RN 92468-67-2 HCAPLUS
CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

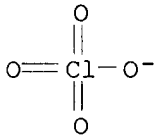
CM 1

CRN 92468-66-1
CMF C60 H77 Fe2 P4 Rh2
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4



L104 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:215759 HCAPLUS
DN 98:215759
ED Entered STN: 12 May 1984
TI Structure of the **hydrogenation** catalyst [(PP)**Rh**(NBD)]ClO4, PP = (η5-(Me3C)2PC5H4)2Fe, and some comparative rate studies
AU Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W. B.; Jones, Terry
CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
SO Organometallics (**1983**), 2(6), 714-19
CODEN: ORGND7; ISSN: 0276-7333
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 34, 75
GI For diagram(s), see printed CA Issue.
AB In this abstract NBD is norbornadiene. The structure of the homogeneous **hydrogenation** precursor I (R = Me3C).cntdot.**Rh**(NBD)ClO4(II), determined crystallog., shows that **Rh** is in a distorted square planar environment involving both NBD double bonds; the bidentates atoms also chelate the **Rh** atom. The steric and electronic effects of the bis(phosphine) ligands in the ferrocenyl moiety are related to the relative **hydrogenation** kinetics of CH2:CRCO2H (R = NHAc, CH2CO2H) or PhCH:CRCO2H (R = NHAc, Me) in EtOH or MeOH containing II or I (R = Ph).cntdot.**Rh**(NBD)ClO4. The mechanism was discussed.
ST crystal structure **rhodium** phosphinoferrocene complex; mol

structure **rhodium** norbornadiene complex; **hydrogenation** catalyst **rhodium** complex; kinetics **hydrogenation** acetamidoacrylic acid; mechanism hydration catalyst acetamidoacrylic acid; acetamidocinnamic acid kinetics **hydrogenation**; itaconic acid kinetics **hydrogenation**; steric effect kinetics **hydrogenation**; solvent kinetics **hydrogenation**

IT Ligands
RL: RCT (Reactant); RACT (Reactant or reagent)
(bis(phosphino)ferrocenes, for **rhodium** in homogeneous **hydrogenation** catalyst, substituent effects and)

IT Bond
(in **rhodium** complex homogeneous **hydrogenation** catalyst containing bis(phosphino)ferrocene ligands)

IT Kinetics of **hydrogenation**
(of alkenoic acids in presence of **rhodium** complexes containing bis(phosphino)ferrocenes)

IT **Hydrogenation**
(of alkenoic acids, in presence of **rhodium** complexes containing bis(phosphino)ferrocenes, mechanism of)

IT Crystal structure
Molecular structure
(of **rhodium** complex with bis(phosphino)ferrocene)

IT Steric effect
Substituent effect
(on **hydrogenation** activity of **rhodium** complexes containing bis(phosphino)ferrocenes)

IT Solvent effect
(on **hydrogenation** of alkenoic acids in presence of **rhodium** complexes with bis(phosphino)ferrocenes)

IT **Hydrogenation catalysts**
(**rhodium** complexes containing norbornadiene and bis(phosphino)ferrocenes, for alkenoic acids, kinetics and mechanism with)

IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(unsatd., **hydrogenation** of, in presence of **rhodium** complexes containing bis(phosphino)ferrocenes)

IT **84680-96-6 84680-98-8**
RL: CAT (Catalyst use); USES (Uses)
(**hydrogenation** catalyst, for alkenoic acids, kinetics and mechanism with)

IT 97-65-4, reactions 1199-77-5 5429-56-1 5469-45-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, in presence of **rhodium** complexes with norbornadiene and bis(phosphino)ferrocenes, kinetics and mechanism of)

IT **84680-95-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with **rhodium** and norbornadiene)

IT 11106-52-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorodibutylphosphine)

IT 13716-10-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dilithioferrocenebis(tetramethylethylenediamine))

IT **84680-96-6 84680-98-8**
RL: CAT (Catalyst use); USES (Uses)
(**hydrogenation** catalyst, for alkenoic acids, kinetics and mechanism with)

RN 84680-96-6 HCAPLUS

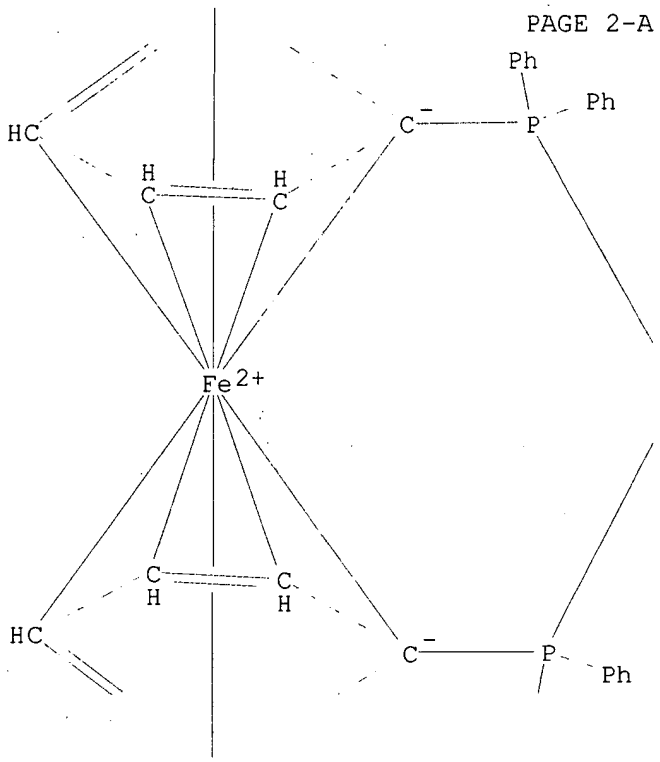
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

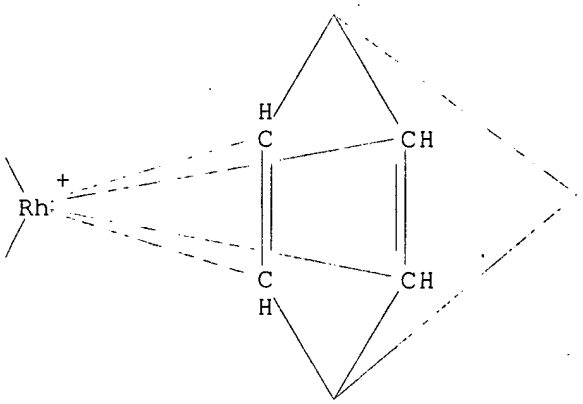
CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



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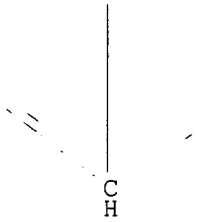

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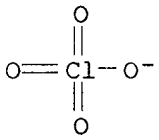
CRN 14797-73-0
CMF Cl O4



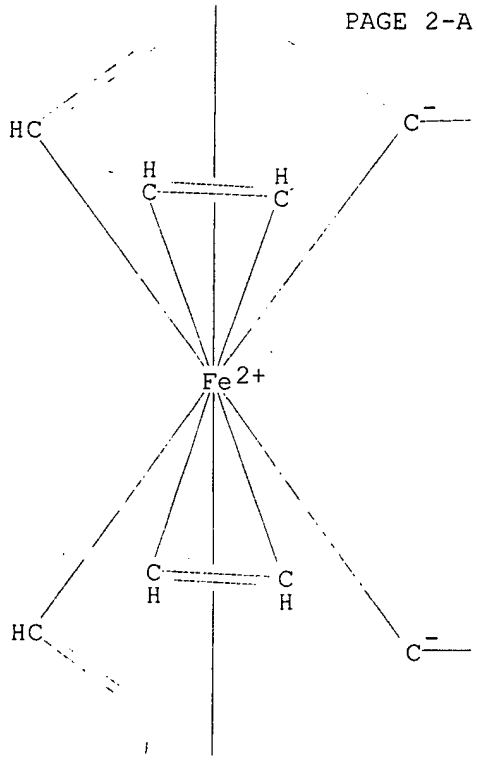
RN 84680-98-8 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 84680-97-7
CMF C33 H52 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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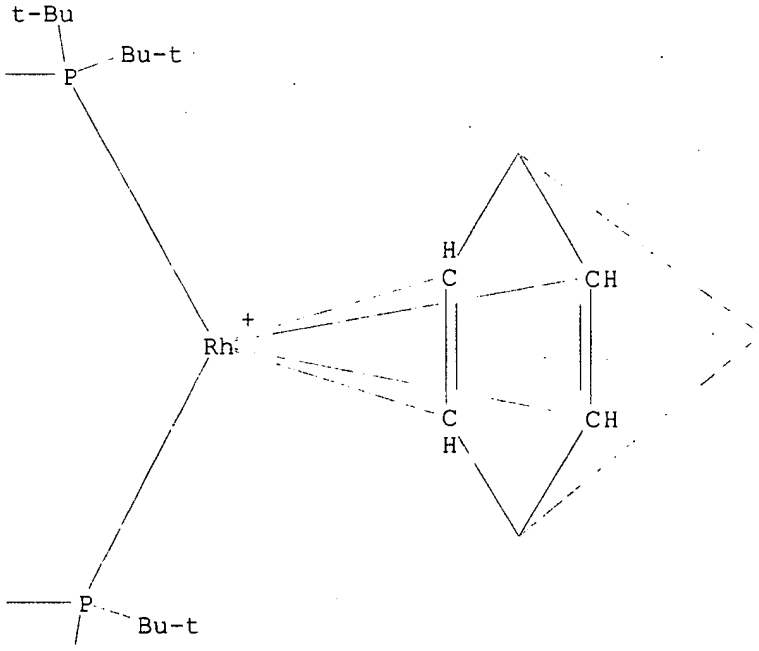

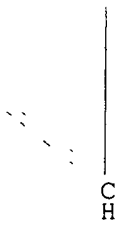

PAGE 3-A

PAGE 3-B

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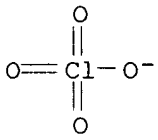
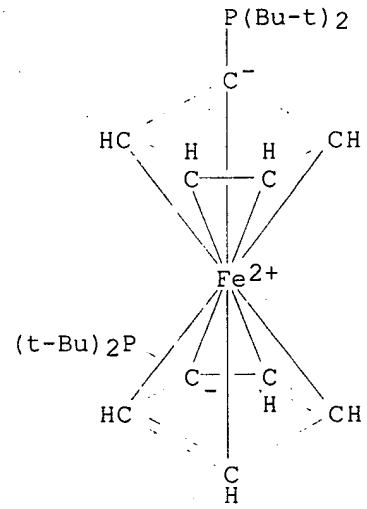
CM 2

CRN 14797-73-0
CMF Cl O4



IT **84680-95-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with **rhodium** and norbornadiene)
RN 84680-95-5 HCAPLUS
CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]- (9CI) (CA INDEX NAME)



L104 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:610374 HCAPLUS

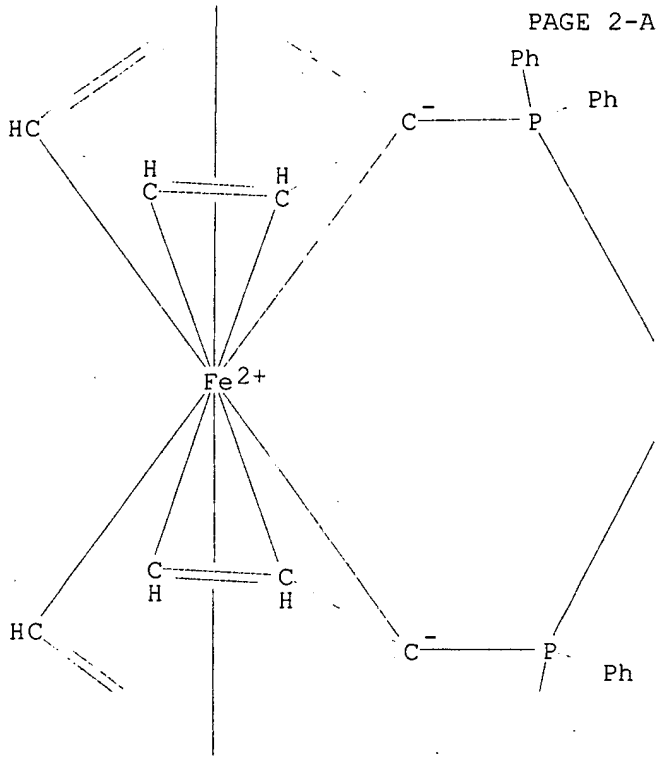
DN 95:210374
ED Entered STN: 12 May 1984
TI The mechanism of asymmetric homogeneous hydrogenation. Solvent complexes and dihydrides from rhodium diphosphine precursors
AU Brown, John M.; Chaloner, Penny A.; Kent, Alexander G.; Murrer, Barry A.; Nicholson, Philip N.; Parker, David; Sidebottom, Philip J.
CS Dyson Perrins Lab., Oxford, OX1 3QY, UK
SO Journal of Organometallic Chemistry (**1981**), 216(2), 263-76
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
CC 67-1 (Catalysis and Reaction Kinetics)
Section cross-reference(s): 22
AB Bicyclo[2.2.1]hepta-2,5-diene and cycloocta-1,5 diene(biphosphine)Rh tetrafluoroborates react with H at 1 atm in methanol or other polar solvents to give as initial product either a solvated dihydride or a solvate. Depending on phosphine structure the equilibrium between these 2 species varies widely. Dihydrides are normally the stable product when the ligand is a monophosphine although (o-methoxyphenyl)methylphenylphosphine is an exception. Cis Chelating biphosphines normally form solvate complexes with no affinity for H. R-Ph bis(diphenylphosphinoethane) falls into this category, but the 31P NMR spectra of its complexes demonstrate an equilibrium between monomeric and dimeric species, and addition of triethylamine gives rise to a trimer. Trans-Chelating biphosphines show more variable behavior, and in the case of bis-1,5-diphenylphosphinopentane, a number of complexes, including one requiring C-H activation, were observed
ST hydrogenation catalyst rhodium phosphine olefin; bicycloheptadiene rhodium phosphine hydrogenation catalyst; cycloctadiene rhodium phosphine hydrogenation catalyst
IT Hydrogenation catalysts
(rhodium bicycloheptadiene by phosphinetetrafluoroborates, solvent complexes and dihydrides of)
IT 79790-95-7
RL: CAT (Catalyst use); USES (Uses)
(hydrogenation catalysts, preparation of solvent complexes and dihydrides of)
IT 34664-30-7 34664-31-8 60430-43-5 60584-05-6 65606-90-8
68811-61-0 68811-82-5 74498-00-3 75085-38-0 79255-71-3
79790-89-9 79790-91-3 **79790-98-0** 79795-96-3
RL: CAT (Catalyst use); USES (Uses)
(hydrogenation catalysts, solvent complexes and dihydrides of)
IT 69381-91-5P 121902-83-8P
RL: PREP (Preparation)
(preparation of)
IT **79790-98-0**
RL: CAT (Catalyst use); USES (Uses)
(hydrogenation catalysts, solvent complexes and dihydrides of)
RN 79790-98-0 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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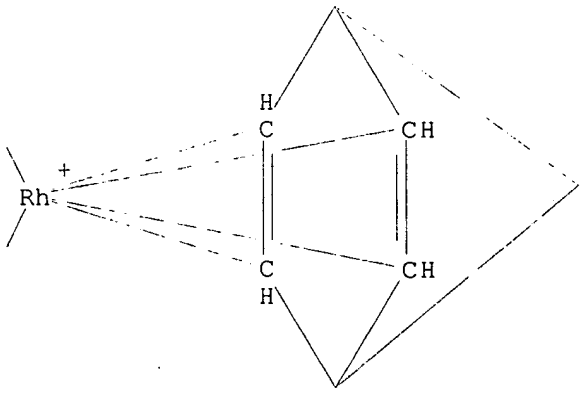
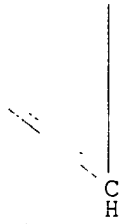
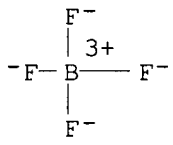




PAGE 3-A
Ph

CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



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